Cycloheptyl isopropylphosphonofluoridate

Inchi: InChI=1S/C10H20FO2P/c1-9(2)14(11,12)13-10-7-5-3-4-6-8-10/h9-10H,3-8H2,1-2H3
InchiKey: NUCIKSFHUMHTLN-UHFFFAOYSA-N
Formula: C10H20FO2P
SMILES: CC(C)P(=O)(F)OC1CCCCCC1
Mol. weight [g/mol]: 222.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.34		Crippen Method
logp	4.297		Crippen Method
mcvol	174.870	ml/mol	McGowan Method
rinpol	1490.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U298272&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