Cycloheptyl propylphosphonofluoridoate

Other names: Cycloheptyl propylphosphonofluoridate
Inchi: InChI=1S/C10H20FO2P/c1-2-9-14(11,12)13-10-7-5-3-4-6-8-10/h10H,2-9H2,1H3
InchiKey: QQPJTWHNYFSLKY-UHFFFAOYSA-N
Formula: C10H20FO2P
SMILES: CCCP(=O)(F)OC1CCCCCC1
Mol. weight [g/mol]: 222.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	4.298		Crippen Method
mcvol	174.870	ml/mol	McGowan Method
rinpol	1528.00		NIST Webbook
rinpol	1528.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U298297&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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