Cyclopentyl propylphosphonofluoridate

Inchi: InChI=1S/C8H16FO2P/c1-2-7-12(9,10)11-8-5-3-4-6-8/h8H,2-7H2,1H3
InchiKey: ADZXLTKPISPAKG-UHFFFAOYSA-N
Formula: C8H16FO2P
SMILES: CCCP(=O)(F)OC1CCCC1
Mol. weight [g/mol]: 194.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	3.518		Crippen Method
mcvol	146.690	ml/mol	McGowan Method
rinpol	1289.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U298288&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