Phosphonofluoridic acid, ethyl-, cyclopentyl ester

Other names: Cyclopentyl ehtylphosphonofluoridate
Cyclopentyl ethylphosphonofluoridate
Inchi: InChI=1S/C7H14FO2P/c1-2-11(8,9)10-7-5-3-4-6-7/h7H,2-6H2,1H3
InchiKey: BMYQDWCAODOERJ-UHFFFAOYSA-N
Formula: C7H14FO2P
SMILES: CCP(=O)(F)OC1CCCC1
Mol. weight [g/mol]: 180.16
CAS: 345239-06-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Crippen Method
logp	3.128		Crippen Method
mcvol	132.600	ml/mol	McGowan Method
rinpol	1199.00		NIST Webbook
rinpol	1199.00		NIST Webbook

Sources

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=C345239067&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices