

Cyclohexyl propylphosphonofluoridate

Inchi: InChI=1S/C9H18FO2P/c1-2-8-13(10,11)12-9-6-4-3-5-7-9/h9H,2-8H2,1H3
InchiKey: CGXBQJDGKMGTRV-UHFFFAOYSA-N
Formula: C9H18FO2P
SMILES: CCCP(=O)(F)OC1CCCCC1
Mol. weight [g/mol]: 208.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.81		Crippen Method
logp	3.908		Crippen Method
mcvol	160.780	ml/mol	McGowan Method
rinpol	1394.00		NIST Webbook
rinpol	1394.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U298441&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

Latest version available from:

<https://www.cheméo.com/cid/119-400-5/Cyclohexyl-propylphosphonofluoridate.pdf>

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