Phosphonofluoridic acid, 2-methylcyclohexyl ester

Other names: 2-Methylcyclohexyl methylphosphonofluoridate
Phosphonofluoridic acid, 2-methylcyclohexyl ester
Methylphosphonic acid, fluoroanhydride, 2-methylcyclohexyl ester
2-methylcyclohexyl methylphosphonofluorid

Inchi: InChI=1S/C8H16FO2P/c1-7-5-3-4-6-8(7)11-12(2,9)10/h7-8H,3-6H2,1-2H3

InchiKey: YBZCCTLVJWWETH-UHFFFAOYSA-N

Formula: C8H16FO2P

SMILES: CC1CCCCC1OP(C)(=O)F

Mol. weight [g/mol]: 194.19

Physical Properties

Property code	Value	Unit	Source
logp	3.374		Crippen Method
mcvol	146.690	ml/mol	McGowan Method
rinpol	1262.00		NIST Webbook
rinpol	1210.20		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1211.70		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1261.70		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1211.70		NIST Webbook
rinpol	1256.70		NIST Webbook
rinpol	1258.50		NIST Webbook
rinpol	1261.70		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1262.00		NIST Webbook
ripol	1790.20		NIST Webbook
ripol	1784.60		NIST Webbook
ripol	1784.60		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85473321&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices