

Phosphonofluoridic acid, (1-methylethyl)-, cyclohexyl ester

Other names:	Cyclohexyl isopropylphosphonofluoridate
Inchi:	InChI=1S/C9H18FO2P/c1-8(2)13(10,11)12-9-6-4-3-5-7-9/h8-9H,3-7H2,1-2H3
InchiKey:	BSSKRMAEPPGXAO-UHFFFAOYSA-N
Formula:	C9H18FO2P
SMILES:	CC(C)P(=O)(F)OC1CCCCC1
Mol. weight [g/mol]:	208.21
CAS:	333416-55-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	3.907		Crippen Method
mcvol	160.780	ml/mol	McGowan Method
rinpol	1357.00		NIST Webbook
rinpol	1357.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C333416550&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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