

n-Pentyl methylphosphonofluoridate

Other names:	Pentyl methylphosphonofluoridate Methylphosphonic acid, fluoroanhydride, penthyl ester Phosphonofluoridic acid, P-methyl-, pentyl ester
Inchi:	InChI=1S/C6H14FO2P/c1-3-4-5-6-9-10(2,7)8/h3-6H2,1-2H3
InchiKey:	DCTCNMMFVAJVCF-UHFFFAOYSA-N
Formula:	C6H14FO2P
SMILES:	CCCCCOP(C)(=O)F
Mol. weight [g/mol]:	168.15
CAS:	13454-59-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.55		Crippen Method
logp	2.986		Crippen Method
mcvol	129.370	ml/mol	McGowan Method
rinpol	1073.00		NIST Webbook
rinpol	1073.40		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1073.40		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13454596&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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