

n-Hexyl methylphosphonofluoridate

Other names:	Hexyl methylphosphonofluoridate Methylphosphonic acid, fluoroanhydride, hexyl ester
Inchi:	InChI=1S/C7H16FO2P/c1-3-4-5-6-7-10-11(2,8)9/h3-7H2,1-2H3
InchiKey:	IPRNMZIRVLGZQD-UHFFFAOYSA-N
Formula:	C7H16FO2P
SMILES:	CCCCCOP(C)(=O)F
Mol. weight [g/mol]:	182.17
CAS:	113548-89-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Crippen Method
logp	3.376		Crippen Method
mcvol	143.460	ml/mol	McGowan Method
rinpol	1172.00		NIST Webbook
rinpol	1171.50		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1172.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C113548893&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

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