

Butyl ethylphosphonofluoridate

Other names:	Phosphonofluoridic acid, ethyl-, butyl ester Ethylphoshonic acid, fluoroanhydride, butyl ester
Inchi:	InChI=1S/C6H14FO2P/c1-3-5-6-9-10(7,8)4-2/h3-6H2,1-2H3
InchiKey:	UOJXJGNUFSBSJG-UHFFFAOYSA-N
Formula:	C6H14FO2P
SMILES:	CCCCOP(=O)(F)CC
Mol. weight [g/mol]:	168.15
CAS:	18358-34-4

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	1067.00		NIST Webbook
rinpol	1067.20		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1067.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18358344&Units=SI
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

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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<https://www.chemeo.com/cid/64-021-7/Butyl-ethylphosphonofluoridate.pdf>

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