

# 2-Butyl ethylphosphonofluoridate

<b>Other names:</b>	Ethylphosphonic acid, fluoroanhydride, 1-methylpropyl ester Sec-butyl ethylphosphonofluoridate s-butyl ethylphosphonofluoridate
<b>Inchi:</b>	InChI=1S/C6H14FO2P/c1-4-6(3)9-10(7,8)5-2/h6H,4-5H2,1-3H3
<b>InchiKey:</b>	XUDFVXLCFULGLL-UHFFFAOYSA-N
<b>Formula:</b>	C6H14FO2P
<b>SMILES:</b>	CCC(C)OP(=O)(F)CC
<b>Mol. weight [g/mol]:</b>	168.15
<b>CAS:</b>	162085-83-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Crippen Method
logp	2.984		Crippen Method
mcvol	129.370	ml/mol	McGowan Method
rinpol	1015.00		NIST Webbook
rinpol	1015.00		NIST Webbook
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rinpol	1015.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C162085838&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C162085838&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

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