

# 2-Butyl methylphosphonofluoridate

<b>Other names:</b>	Sec-butyl methylphosphonofluoridate S-Butyl methylphosphonofluoridate 1-Methylpropyl methylphosphonofluoridate
<b>Inchi:</b>	InChI=1S/C5H12FO2P/c1-4-5(2)8-9(3,6)7/h5H,4H2,1-3H3
<b>InchiKey:</b>	INIUKZAEJHEEFF-UHFFFAOYSA-N
<b>Formula:</b>	C5H12FO2P
<b>SMILES:</b>	CCC(C)OP(C)(=O)F
<b>Mol. weight [g/mol]:</b>	154.12
<b>CAS:</b>	352-52-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	2.594		Crippen Method
mcvol	115.280	ml/mol	McGowan Method
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	917.90		NIST Webbook
rinpol	918.00		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=C352523&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C352523&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

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