

# Isobutyl ethylphosphonofluoridate

<b>Other names:</b>	Posphonofluoridic acid, ethyl-, isobutyl ester Ethylphoshonic acid, fluoroanhydride, 2-methylpropyl ester Isobutyl ethylphosphonofluoridoate Phosphonofluoridic acid, P-ethyl-, 2-methylpropyl ester
<b>Inchi:</b>	InChI=1S/C6H14FO2P/c1-4-10(7,8)9-5-6(2)3/h6H,4-5H2,1-3H3
<b>InchiKey:</b>	ZAERZDLQUJPTPS-UHFFFAOYSA-N
<b>Formula:</b>	C6H14FO2P
<b>SMILES:</b>	CCP(=O)(F)OCC(C)C
<b>Mol. weight [g/mol]:</b>	168.15
<b>CAS:</b>	2261-83-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	2.841		Crippen Method
mcvol	129.370	ml/mol	McGowan Method
rinpol	1028.00		NIST Webbook
rinpol	1027.70		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1027.70		NIST Webbook

## Sources

<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=C2261838&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2261838&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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