

# Isobutyl methylphosphonic acid, TMS derivative

<b>Other names:</b>	Methylphosphonic acid, isobutyl ester, TMS Methylphosphonic acid, isobutyl trimethylsilyl ester Methylphosphonic acid, mono-isobutyl ester, TMS
<b>Inchi:</b>	InChI=1S/C8H21O3PSi/c1-8(2)7-10-12(3,9)11-13(4,5)6/h8H,7H2,1-6H3
<b>InchiKey:</b>	YKENHQTWUXRYMG-UHFFFAOYSA-N
<b>Formula:</b>	C8H21O3PSi
<b>SMILES:</b>	CC(C)COP(C)(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	224.31
<b>CAS:</b>	199116-09-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	3.333		Crippen Method
rinpol	1214.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1221.00		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>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C199116091&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C199116091&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
<b>rinpol:</b>	Non-polar retention indices

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