

# 2-Methylcyclosarin

<b>Other names:</b>	2-Methylcyclohexyl methylphosphonofluoridate Phosphonofluoridic acid, 2-methylcyclohexyl ester Methylphosphonic acid, fluoroanhydride, 2-methylcyclohexyl ester 2-methylcyclohexyl methylphosphonofluorid
<b>Inchi:</b>	InChI=1S/C8H16FO2P/c1-7-5-3-4-6-8(7)11-12(2,9)10/h7-8H,3-6H2,1-2H3
<b>InchiKey:</b>	YBZCCTLVJWWETH-UHFFFAOYSA-N
<b>Formula:</b>	C8H16FO2P
<b>SMILES:</b>	CC1CCCCC1OP(C)(=O)F
<b>Mol. weight [g/mol]:</b>	194.18
<b>CAS:</b>	85473-32-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.15		Crippen Method
logp	3.374		Crippen Method
mcvol	146.690	ml/mol	McGowan Method
rinpol	1210.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1210.20		NIST Webbook
rinpol	1211.70		NIST Webbook
rinpol	1256.70		NIST Webbook
rinpol	1258.50		NIST Webbook
rinpol	1261.70		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1211.70		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1261.70		NIST Webbook
rinpol	1262.00		NIST Webbook
ripol	1784.60		NIST Webbook
ripol	1790.20		NIST Webbook
ripol	1784.60		NIST Webbook

# Sources

<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>
<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=C85473321&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C85473321&amp;Units=SI</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
<b>ripol:</b>	Polar retention indices

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