

# 9H-Purine, 6-chloro-9-(methoxymethyl)-

<b>Other names:</b>	6-Chloro-9-methoxymethylpurine
<b>Inchi:</b>	InChI=1S/C7H7ClN4O/c1-13-4-12-3-11-5-6(8)9-2-10-7(5)12/h2-3H,4H2,1H3
<b>InchiKey:</b>	SZLMRHFSYVCXQX-UHFFFAOYSA-N
<b>Formula:</b>	C7H7ClN4O
<b>SMILES:</b>	COCn1cnc2c(Cl)ncnc21
<b>Mol. weight [g/mol]:</b>	198.61
<b>CAS:</b>	6504-64-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	1.084		Crippen Method
mcvol	128.600	ml/mol	McGowan Method

## 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=C6504649&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6504649&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>mcvol:</b>	McGowan's characteristic volume

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