

# Adenine, 2-chloro-

<b>Other names:</b>	9H-Purin-6-amine, 2-chloro-2-chloroadenine
<b>Inchi:</b>	InChI=1S/C5H4ClN5/c6-5-10-3(7)2-4(11-5)9-1-8-2/h1H,(H3,7,8,9,10,11)
<b>InchiKey:</b>	HBJGQJWNMZDFKL-UHFFFAOYSA-N
<b>Formula:</b>	C5H4ClN5
<b>SMILES:</b>	<chem>Nc1nc(Cl)nc2[nH]cnc12</chem>
<b>Mol. weight [g/mol]:</b>	169.57
<b>CAS:</b>	1839-18-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	0.107		Crippen Method
mcvol	104.530	ml/mol	McGowan Method

## 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=C1839185&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1839185&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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