

# Indole-3-acetic acid, 4-chloro-2-methyl-

<b>Inchi:</b>	InChI=1S/C11H10ClNO2/c1-6-7(5-10(14)15)11-8(12)3-2-4-9(11)13-6/h2-4,13H,5H2,1H3
<b>InchiKey:</b>	DVYFYFAMPUDXFH-UHFFFAOYSA-N
<b>Formula:</b>	C11H10ClNO2
<b>SMILES:</b>	<chem>Cc1[nH]c2cccc(Cl)c2c1CC(=O)O</chem>
<b>Mol. weight [g/mol]:</b>	223.66
<b>CAS:</b>	6127-20-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	2.275		Crippen Method
mcvol	156.590	ml/mol	McGowan Method

## Sources

<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>
<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=C6127204&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6127204&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

Latest version available from:

<https://www.chemeo.com/cid/115-520-6/Indole-3-acetic-acid-4-chloro-2-methyl.pdf>

Generated by Cheméo on 2024-05-06 07:33:11.920587727 +0000 UTC m=+17270040.841165043.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.