

# 5-Chloro-2-piperidyl-acetanilide

<b>Inchi:</b>	InChI=1S/C13H17ClN2O/c1-10(17)15-12-9-11(14)5-6-13(12)16-7-3-2-4-8-16/h5-6,9H,2-4
<b>InchiKey:</b>	MNQXXDBLEOCASW-UHFFFAOYSA-N
<b>Formula:</b>	C13H17ClN2O
<b>SMILES:</b>	CC(=O)Nc1cc(Cl)ccc1N1CCCCC1
<b>Mol. weight [g/mol]:</b>	252.74
<b>CAS:</b>	116495-98-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	3.289		Crippen Method
mcvol	193.180	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=C116495988&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116495988&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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