

# Nicotinamide, N-(3-chlorophenyl)-

<b>Inchi:</b>	InChI=1S/C12H9ClN2O/c13-10-4-1-5-11(7-10)15-12(16)9-3-2-6-14-8-9/h1-8H,(H,15,16)
<b>InchiKey:</b>	XQPPPWLPXGVYAJ-UHFFFAOYSA-N
<b>Formula:</b>	C12H9ClN2O
<b>SMILES:</b>	O=C(Nc1cccc(Cl)c1)c1cccnc1
<b>Mol. weight [g/mol]:</b>	232.67

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	2.987		Crippen Method
mcvol	166.190	ml/mol	McGowan Method
rinpol	2181.00		NIST Webbook

## 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=U308106&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308106&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
<b>rinpol:</b>	Non-polar retention indices

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