

# 4-Chloroquinoline

<b>Other names:</b>	Quinoline, 4-chloro-
<b>Inchi:</b>	InChI=1S/C9H6ClN/c10-8-5-6-11-9-4-2-1-3-7(8)9/h1-6H
<b>InchiKey:</b>	KNDOFJFSHZCKGT-UHFFFAOYSA-N
<b>Formula:</b>	C9H6ClN
<b>SMILES:</b>	Clc1ccnc2ccccc12
<b>Mol. weight [g/mol]:</b>	163.60
<b>CAS:</b>	611-35-8

## Physical Properties

Property code	Value	Unit	Source
hsub	78.60 ± 1.70	kJ/mol	NIST Webbook
log10ws	-3.73		Crippen Method
logp	2.888		Crippen Method
mcvol	116.670	ml/mol	McGowan Method
tb	533.70	K	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=C611358&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C611358&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>hsub:</b>	Enthalpy of sublimation at standard conditions
<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>tb:</b>	Normal Boiling Point Temperature

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