

# Pyrimidine, 2-chloro-

<b>Other names:</b>	2-Chloropyrimidine
<b>Inchi:</b>	InChI=1S/C4H3ClN2/c5-4-6-2-1-3-7-4/h1-3H
<b>InchiKey:</b>	UNCQVRBWJWWJBF-UHFFFAOYSA-N
<b>Formula:</b>	C4H3ClN2
<b>SMILES:</b>	Clc1ncccn1
<b>Mol. weight [g/mol]:</b>	114.53
<b>CAS:</b>	1722-12-9

## Physical Properties

Property code	Value	Unit	Source
hsub	70.10 ± 1.30	kJ/mol	NIST Webbook
log10ws	-1.69		Crippen Method
logp	1.130		Crippen Method
mvol	75.660	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.70	K	1.30	NIST Webbook

## 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=C1722129&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1722129&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>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>tbrp:</b>	Boiling point at reduced pressure

Latest version available from:

<https://www.cheméo.com/cid/69-088-9/Pyrimidine-2-chloro.pdf>

Generated by Cheméo on 2024-04-27 09:55:58.78589277 +0000 UTC m=+16501007.706470086.

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