Pyrimidine, 2-chloro-

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1722129&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure