

4-Chloropyridine

Other names:	Pyridine, 4-chloro- p-Chloropyridine
Inchi:	InChI=1S/C5H4ClN/c6-5-1-3-7-4-2-5/h1-4H
InchiKey:	PVMNPAUTCMBOMO-UHFFFAOYSA-N
Formula:	C5H4ClN
SMILES:	Clc1ccncc1
Mol. weight [g/mol]:	113.55
CAS:	626-61-9

Physical Properties

Property code	Value	Unit	Source
affp	916.10	kJ/mol	NIST Webbook
basg	884.20	kJ/mol	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	10.15 ± 0.05	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	9.86	eV	NIST Webbook
log10ws	-1.92		Crippen Method
logp	1.735		Crippen Method
mcvol	79.770	ml/mol	McGowan Method
tb	420.70	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.20	K	13.30	NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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=C626619&Units=SI>

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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