Pyridine, 2-chloro-

Other names:	2-Chloropyridine
	ALPHA-CHLOROPYRIDINE
	O-CHLOROPYRIDINE
	UN 2822
	«alpha»-Chloropyridine
	Â«alphaÂ»-Chloropyridine
Inchi:	InChI=1S/C5H4ClN/c6-5-3-1-2-4-7-5/h1-4H
InchiKey:	OKDGRDCXVWSXDC-UHFFFAOYSA-N
Formula:	C5H4ClN
SMILES:	Clc1ccccn1
Mol. weight [g/mol]:	113.55
CAS:	109-09-1

Physical Properties

Property code	Value	Unit	Source
affp	900.90	kJ/mol	NIST Webbook
basg	869.00	kJ/mol	NIST Webbook
hvap	51.00 ± 1.20	kJ/mol	NIST Webbook
ie	9.91 ± 0.05	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.90 ± 0.10	eV	NIST Webbook
ie	9.68	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-1.92		Crippen Method
logp	1.735		Crippen Method
mcvol	79.770	ml/mol	McGowan Method
rinpol	895.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	900.00		NIST Webbook
tb	443.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	53.00	kJ/mol	365.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	439.20	K	95.20	NIST Webbook
tbrp	329.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58408e+01
Coeff. B	-4.78999e+03
Coeff. C	-1.63770e+01
Temperature range (K), min.	324.35
Temperature range (K), max.	471.30

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1789.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109091&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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