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

Physical Properties

Property code	Value	Unit	Source
af	0.2722		Cheméo Relay (1.0)
affp	916.10	kJ/mol	NIST Webbook
basg	884.20	kJ/mol	NIST Webbook
gf	150.93	kJ/mol	Cheméo Relay (1.0, beta)
hf	102.02	kJ/mol	Cheméo Relay (1.0)
hvap	49.35	kJ/mol	Cheméo Relay (1.0)
ie	10.10	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	9.86	eV	NIST Webbook
ie	10.15 ± 0.05	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
log10ws	-0.19		Cheméo Relay (1.0)
logp	1.735		Crippen Method
mcvol	79.770	ml/mol	McGowan Method
pc	5206.96	kPa	Cheméo Relay (1.0, beta)
tb	420.70	K	NIST Webbook
tc	671.41	K	Cheméo Relay (1.0)
tf	320.39	K	Cheméo Relay (1.0)
vc	0.275	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

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

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C626619&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume