Pyridine, 3-chloro-

Other names: m-Chloropyridine
3-Chloropyridine
«beta»-Chloropyridine
Inchi: InChI=1S/C5H4ClN/c6-5-2-1-3-7-4-5/h1-4H
InchiKey: PWRBCZZQRRPXAB-UHFFFAOYSA-N
Formula: C5H4ClN
SMILES: Clc1cccnc1
Mol. weight [g/mol]: 113.55
CAS: 626-60-8

Physical Properties

Property code	Value	Unit	Source
affp	903.40	kJ/mol	NIST Webbook
basg	871.50	kJ/mol	NIST Webbook
hvap	47.90 ± 1.10	kJ/mol	NIST Webbook
ie	9.58	eV	NIST Webbook
ie	9.65	eV	NIST Webbook
ie	9.80 ± 0.10	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	-1.92		Crippen Method
logp	1.735		Crippen Method
mcvol	79.770	ml/mol	McGowan Method
rinpol	890.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	861.10		NIST Webbook
rinpol	884.50		NIST Webbook
tb	421.20	K	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C626608&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature