

2-Chloro-3-pyridinol

Other names:	2-chloro-3-hydroxypyridine 2-chloropyridin-3-ol 3-Pyridinol, 2-chloro- 3-hydroxy-2-chloropyridine
Inchi:	InChI=1S/C5H4ClNO/c6-5-4(8)2-1-3-7-5/h1-3,8H
InchiKey:	RSOPTYAZDFSMTN-UHFFFAOYSA-N
Formula:	C5H4ClNO
SMILES:	Oc1cccnc1Cl
Mol. weight [g/mol]:	129.54
CAS:	6636-78-8

Physical Properties

Property code	Value	Unit	Source
hfus	26.75	kJ/mol	Structure and energetics correlations in some chlorohydroxypyridines
log10ws	-1.47		Crippen Method
logp	1.441		Crippen Method
mvol	85.640	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Structure and energetics correlations in some chlorohydroxypyridines:	https://www.doi.org/10.1016/j.jct.2013.03.001
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6636788&Units=SI

Legend

hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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