

6-Chloro-2-pyridinol

Other names:	2(1H)-pyridinone, 6-chloro- 2(1H)-pyridone, 6-chloro- 2-chloro-6-hydroxypyridine 6-chloro-2(1H)-pyridinone 6-chloro-2(1H)-pyridone 6-chloro-2-hydroxypyridine 6-chloro-2-pyridone 6-chloropyridin-2-ol
Inchi:	InChI=1S/C5H4ClNO/c6-4-2-1-3-5(8)7-4/h1-3H,(H,7,8)
InchiKey:	CLNNBQDAAGDAHI-UHFFFAOYSA-N
Formula:	C5H4ClNO
SMILES:	Oc1cccc(Cl)n1
Mol. weight [g/mol]:	129.54
CAS:	16879-02-0

Physical Properties

Property code	Value	Unit	Source
hfus	18.38	kJ/mol	Structure and energetics correlations in some chlorohydroxypyridines
log10ws	-1.47		Crippen Method
logp	1.441		Crippen Method
mcvol	85.640	ml/mol	McGowan Method

Sources

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=C16879020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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