4-AMINO-2-CHLOROPYRIDINE

Other names: 2-chloropyridin-4-amine
4-Pyridinamine, 2-chloro-
Inchi: InChI=1S/C5H5ClN2/c6-5-3-4(7)1-2-8-5/h1-3H,(H2,7,8)
InchiKey: BLBDTBCGPHPIJK-UHFFFAOYSA-N
Formula: C5H5ClN2
SMILES: Nc1ccnc(Cl)c1
Mol. weight [g/mol]: 128.56

Physical Properties

Property code	Value	Unit	Source
hvap	62.52	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-0.86		Cheméo Relay (1.0)
logp	1.317		Crippen Method
mcvol	89.750	ml/mol	McGowan Method
tb	528.01	K	Cheméo Relay (1.0)
tf	396.73	K	Cheméo Relay (1.0)

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14432123&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point