Quinoline, 2-chloro-

Other names: 2-Chloroquinoline
Inchi: InChI=1S/C9H6ClN/c10-9-6-5-7-3-1-2-4-8(7)11-9/h1-6H
InchiKey: OFUFXTHGZWIDDB-UHFFFAOYSA-N
Formula: C9H6ClN
SMILES: Clc1ccc2ccccc2n1
Mol. weight [g/mol]: 163.60
CAS: 612-62-4

Physical Properties

Property code	Value	Unit	Source
hsub	84.30 ± 2.60	kJ/mol	NIST Webbook
log10ws	-3.73		Crippen Method
logp	2.888		Crippen Method
mcvol	116.670	ml/mol	McGowan Method
tb	539.70	K	NIST Webbook
tf	403.15 ± 1.50	K	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C612624&Units=SI

Legend

hsub: Enthalpy of sublimation at standard conditions
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