4-Chloroquinoline

Other names:	Quinoline, 4-chloro-
Inchi:	InChI=1S/C9H6ClN/c10-8-5-6-11-9-4-2-1-3-7(8)9/h1-6H
InchiKey:	KNDOFJFSHZCKGT-UHFFFAOYSA-N
Formula:	C9H6ClN
SMILES:	Clc1ccnc2ccccc12
Mol. weight [g/mol]:	163.60
CAS:	611-35-8

Physical Properties

Property code	Value	Unit	Source
hsub	78.60 ± 1.70	kJ/mol	NIST Webbook
log10ws	-3.73		Crippen Method
logp	2.888		Crippen Method
mcvol	116.670	ml/mol	McGowan Method
tb	533.70	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=C611358&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

Latest version available from:

https://www.chemeo.com/cid/54-356-7/4-Chloroquinoline.pdf

Generated by Cheméo on 2024-10-12 06:12:26.928637673 +0000 UTC m=+3294409.565606920.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.