Quinoline, 5-chloro-

Other names:	5-Chloroquinoline
Inchi:	InChI=1S/C9H6ClN/c10-8-4-1-5-9-7(8)3-2-6-11-9/h1-6H
InchiKey:	HJSRGOVAIOPERP-UHFFFAOYSA-N
Formula:	C9H6ClN
SMILES:	Clc1cccc2ncccc12
Mol. weight [g/mol]:	163.60
CAS:	635-27-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Crippen Method
logp	2.888		Crippen Method
mcvol	116.670	ml/mol	McGowan Method
tf	316.00 ± 3.00	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=C635278&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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