4-Chloroquinaldine

Other names:	Quinoline, 4-chloro-2-methyl- Quinaldine, 4-chloro- 4-Chloro-2-methylquinoline
Inchi:	InChI=1S/C10H8ClN/c1-7-6-9(11)8-4-2-3-5-10(8)12-7/h2-6H,1H3
InchiKey:	HQAIROMRVBVWSK-UHFFFAOYSA-N
Formula:	C10H8ClN
SMILES:	Cc1cc(Cl)c2ccccc2n1
Mol. weight [g/mol]:	177.63
CAS:	4295-06-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	3.197		Crippen Method
mcvol	130.760	ml/mol	McGowan Method
rinpol	1432.10		NIST Webbook
tb	542.70	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4295061&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

tb: Normal Boiling Point Temperature