

3-Quinolinecarboxylic acid, 6-chloro-4-hydroxy-

Inchi:	InChI=1S/C10H6ClNO3/c11-5-1-2-8-6(3-5)9(13)7(4-12-8)10(14)15/h1-4H,(H,12,13)(H,14)
InchiKey:	CDPXSMNKRFLXHU-UHFFFAOYSA-N
Formula:	C10H6ClNO3
SMILES:	O=C(O)c1c[nH]c2ccc(Cl)cc2c1=O
Mol. weight [g/mol]:	223.61
CAS:	35973-14-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	1.398		Crippen Method
mcvol	144.070	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35973149&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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