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/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