4-Hydroxy-3-cyano-7-chloro-quinoline

Inchi: InChI=1S/C10H5ClN2O/c11-7-1-2-8-9(3-7)13-5-6(4-12)10(8)14/h1-3,5H,(H,13,14)
InchiKey: AWSDUPVFXCHALA-UHFFFAOYSA-N
Formula: C10H5ClN2O
SMILES: N#Cc1cnc2cc(Cl)ccc2c1O
Mol. weight [g/mol]: 204.61
CAS: 2458-23-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.63		Crippen Method
logp	2.465		Crippen Method
mcvol	138.010	ml/mol	McGowan Method

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=C2458233&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume