

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

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