

5-Quinolinol

Other names:	5-Hydroxyquinoline quinolin-5-ol
Inchi:	InChI=1S/C9H7NO/c11-9-5-1-4-8-7(9)3-2-6-10-8/h1-6,11H
InchiKey:	GYESAYHWISMZOK-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	Oc1cccc2ncccc12
Mol. weight [g/mol]:	145.16
CAS:	578-67-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Aqueous Solubility Prediction Method
log10ws	-2.54		Estimated Solubility Method
logp	1.940		Crippen Method
mcvol	110.300	ml/mol	McGowan Method
tf	497.00 ± 3.00	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C578676&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

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

tf: Normal melting (fusion) point

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