

6-hydroxyquinoline

Other names:	Quinolin-6-ol
Inchi:	InChI=1S/C9H7NO/c11-8-3-4-9-7(6-8)2-1-5-10-9/h1-6,11H
InchiKey:	OVYWMEWYEJLIER-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	Oc1ccc2ncccc2c1
Mol. weight [g/mol]:	145.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Aqueous Solubility Prediction Method
log10ws	-2.16		Estimated Solubility Method
logp	1.940		Crippen Method
mcvol	110.300	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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

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