

5-Isoquinolinol

Other names:	5-Hydroxyisoquinoline isoquinolin-5-ol
Inchi:	InChI=1S/C9H7NO/c11-9-3-1-2-7-6-10-5-4-8(7)9/h1-6,11H
InchiKey:	CSNXUYRHPXGSJD-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	Oc1cccc2cnccc12
Mol. weight [g/mol]:	145.16
CAS:	2439-04-5

Physical Properties

Property code	Value	Unit	Source
hsub	109.60 ± 2.10	kJ/mol	NIST Webbook
log10ws	-2.59		Crippen Method
logp	1.940		Crippen Method
mcvol	110.300	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2439045&Units=SI

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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