

# 1(2H)-Isoquinolinone

<b>Other names:</b>	Isocarbostyrl Isoquinolin-1-one 1(2H)-Isoquinolone 1-Hydroxyisoquinoline 1-Isoquinolinol
<b>Inchi:</b>	InChI=1S/C9H7NO/c11-9-8-4-2-1-3-7(8)5-6-10-9/h1-6H,(H,10,11)
<b>InchiKey:</b>	VDBNYAPERZTOOF-UHFFFAOYSA-N
<b>Formula:</b>	C9H7NO
<b>SMILES:</b>	Oc1nccc2ccccc12
<b>Mol. weight [g/mol]:</b>	145.16
<b>CAS:</b>	491-30-5

## Physical Properties

Property code	Value	Unit	Source
hsub	113.60 ± 2.20	kJ/mol	NIST Webbook
log10ws	-2.59		Crippen Method
logp	1.940		Crippen Method
mvol	110.300	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C491305&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C491305&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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