

# Benzo[f]isoquinoline

<b>Other names:</b>	5,6-Benzoisoquinoline
<b>Inchi:</b>	InChI=1S/C13H9N/c1-2-4-12-10(3-1)5-6-11-9-14-8-7-13(11)12/h1-9H
<b>InchiKey:</b>	JQXCGCPMGZBMLE-UHFFFAOYSA-N
<b>Formula:</b>	C13H9N
<b>SMILES:</b>	<chem>c1ccc2c(c1)ccc1cnccc12</chem>
<b>Mol. weight [g/mol]:</b>	179.22
<b>CAS:</b>	229-67-4

## Physical Properties

Property code	Value	Unit	Source
ie	8.30 ± 0.10	eV	NIST Webbook
log10ws	-4.85		Crippen Method
logp	3.388		Crippen Method
mcvol	141.330	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=C229674&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C229674&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>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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