

# Indeno(1,2,3-ij)isoquinoline

<b>Other names:</b>	1-Azafluoranthene Indeno[1.2.3-ij]isoquinoline
<b>Inchi:</b>	InChI=1S/C15H9N/c1-2-6-13-11(5-1)12-7-3-4-10-8-9-16-15(13)14(10)12/h1-9H
<b>InchiKey:</b>	XQNXAFHTOWJFTR-UHFFFAOYSA-N
<b>Formula:</b>	C15H9N
<b>SMILES:</b>	<chem>c1ccc2c(c1)-c1cccc3ccnc-2c13</chem>
<b>Mol. weight [g/mol]:</b>	203.24
<b>CAS:</b>	206-56-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	3.882		Crippen Method
mcvol	154.350	ml/mol	McGowan Method
rinpol	348.47		NIST Webbook
rinpol	347.57		NIST Webbook
rinpol	348.17		NIST Webbook
rinpol	348.17		NIST Webbook
tb	661.00	K	NIST Webbook
tf	356.00	K	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C206564&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C206564&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>
<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>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tf:</b>	Normal melting (fusion) point

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