11H-Indeno(1,2-b)quinoline

Other names:	2,3-Benz-4-azafluorene
	2,3-Benzo-4-azafluorene
	4-Aza-2,3-benzofluorene
	5-Aza-11H-benzo[b]fluorene
	11H-Indeno[1.2-b]quinoline
Inchi:	InChI=1S/C16H11N/c1-3-7-14-11(5-1)9-13-10-12-6-2-4-8-15(12)17-16(13)14/h1-8,10H,9
InchiKey:	KUZOQBPSADEASZ-UHFFFAOYSA-N
Formula:	C16H11N
SMILES:	c1ccc2c(c1)Cc1cc3ccccc3nc1-2
Mol. weight [g/mol]:	217.27
CAS:	243-51-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.99		Crippen Method
logp	3.806		Crippen Method
mcvol	168.440	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C243516&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume