Indeno(1,2,3-ij)isoquinoline

Other names:	1-Azafluoranthene
	Indeno[1.2.3-ij]isoquinoline
Inchi:	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
InchiKey:	XQNXAFHTOWJFTR-UHFFFAOYSA-N
Formula:	C15H9N
SMILES:	c1ccc2c(c1)-c1cccc3ccnc-2c13
Mol. weight [g/mol]:	203.24
CAS:	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C206564&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point