5H-Indeno[1,2-b]pyridine

Other names:	4-Azafluorene
	5H-Indeno[1.2-b]pyridine
Inchi:	InChI=1S/C12H9N/c1-2-6-11-9(4-1)8-10-5-3-7-13-12(10)11/h1-7H,8H2
InchiKey:	FWEHZHRUCQRSJP-UHFFFAOYSA-N
Formula:	C12H9N
SMILES:	c1ccc2c(c1)Cc1cccnc1-2
Mol. weight [g/mol]:	167.21
CAS:	244-99-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	2.653		Crippen Method
mcvol	131.540	ml/mol	McGowan Method
rinpol	1653.00		NIST Webbook
rinpol	279.54		NIST Webbook
rinpol	278.75		NIST Webbook
rinpol	279.44		NIST Webbook
rinpol	279.85		NIST Webbook
rinpol	279.31		NIST Webbook
rinpol	279.85		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C244995&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices