

2-Azapyrene

Inchi:	InChI=1S/C15H9N/c1-2-10-4-6-12-8-16-9-13-7-5-11(3-1)14(10)15(12)13/h1-9H
InchiKey:	VXNBYQYOFXSMOE-UHFFFAOYSA-N
Formula:	C15H9N
SMILES:	<chem>c1cc2ccc3cncc4ccc(c1)c2c34</chem>
Mol. weight [g/mol]:	203.24
CAS:	193-98-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.07		Crippen Method
logp	3.979		Crippen Method
mcvol	154.350	ml/mol	McGowan Method
rinpol	362.20		NIST Webbook
rinpol	362.43		NIST Webbook
rinpol	362.43		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=C193986&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

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