11H-Benzo[a]carbazole

Other names:	Benzo[a]carbazole
	1,2-Benzcarbazole
	1,2-Benzocarbazole
	11-Azachrysofluorene
Inchi:	InChI=1S/C16H11N/c1-2-6-12-11(5-1)9-10-14-13-7-3-4-8-15(13)17-16(12)14/h1-10,17H
InchiKey:	MYKQKWIPLZEVOW-UHFFFAOYSA-N
Formula:	C16H11N
SMILES:	c1ccc2c(c1)ccc1c3ccccc3[nH]c21
Mol. weight [g/mol]:	217.27
CAS:	239-01-0

Physical Properties

Property code	Value	Unit	Source
ie	7.10 ± 0.10	eV	NIST Webbook
log10ws	-6.10		Crippen Method
logp	3.992		Crippen Method
mcvol	168.440	ml/mol	McGowan Method
rinpol	403.50		NIST Webbook
rinpol	402.22		NIST Webbook
rinpol	401.81		NIST Webbook
rinpol	400.00		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=C239010&Units=SI

Legend

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