13H-Dibenzo[a,i]carbazole

Other names:	1,2,7,8-Dibenzcarbazole
	1,2:7,8-Dibenzocarbazole
	13-Aza-13H-dibenzo[a,i]fluorene
	13H-dibenzo(a,i)carbazole
	7H-Dibenzo(a,i)carbazole
	dibenzo[a,i]carbazole
Inchi:	InChI=1S/C20H13N/c1-3-7-15-13(5-1)9-11-17-18-12-10-14-6-2-4-8-16(14)20(18)21-19(1
InchiKey:	IUILSTHMSGDSHQ-UHFFFAOYSA-N
Formula:	C20H13N
SMILES:	c1ccc2c(c1)ccc1c3ccc4ccccc4c3[nH]c21
Mol. weight [g/mol]:	267.32
CAS:	239-64-5

Physical Properties

Property code	Value	Unit	Source
ie	7.10 ± 0.10	eV	NIST Webbook
log10ws	-7.42		Aqueous Solubility Prediction Method
logp	5.146		Crippen Method
mcvol	205.340	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C239645&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume