Benzo(c)carbazole

Other names:	1H-Benzo[c]carbazole
	3,4-Benzocarbazole
Inchi:	InChI=1S/C16H11N/c1-2-6-12-11(5-1)9-10-15-16(12)13-7-3-4-8-14(13)17-15/h1-5,7-10H
InchiKey:	CNEBOSRZUQUQMH-UHFFFAOYSA-N
Formula:	C16H11N
SMILES:	C1=CCc2c3c(ccc2=C1)=Nc1ccccc1-3
Mol. weight [g/mol]:	217.27
CAS:	34777-33-8

Physical Properties

Property code	Value	Unit	Source
ie	7.30 ± 0.10	eV	NIST Webbook
log10ws	-4.18		Crippen Method
logp	2.511		Crippen Method
mcvol	168.440	ml/mol	McGowan Method

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=C34777338&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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