

Benzo(b)carbazole

Other names:	5H-Benzo[b]carbazole Benzocarbazole 2,3-Benzcarbazole 2,3-Benzocarbazole
Inchi:	InChI=1S/C16H11N/c1-2-6-12-10-16-14(9-11(12)5-1)13-7-3-4-8-15(13)17-16/h1-10,17H
InchiKey:	ROEOVWIEALGNLM-UHFFFAOYSA-N
Formula:	C16H11N
SMILES:	<chem>c1ccc2cc3c(cc2c1)[nH]c1cccc13</chem>
Mol. weight [g/mol]:	217.27
CAS:	243-28-7

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	2442.00		NIST Webbook
rinpol	410.12		NIST Webbook
rinpol	409.31		NIST Webbook
rinpol	409.31		NIST Webbook
rinpol	410.12		NIST Webbook
rinpol	407.54		NIST Webbook
rinpol	409.63		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C243287&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

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