

5H-Naphtho[2,3-b]carbazole

Other names:	Naphtho[2,3-b]carbazole
Inchi:	InChI=1S/C20H13N/c1-2-6-14-10-16-12-20-18(11-15(16)9-13(14)5-1)17-7-3-4-8-19(17)2
InchiKey:	MEXWZXCQQQYPNG-UHFFFAOYSA-N
Formula:	C20H13N
SMILES:	<chem>c1ccc2cc3cc4c(cc3cc2c1)[nH]c1cccc14</chem>
Mol. weight [g/mol]:	267.32
CAS:	248-96-4

Physical Properties

Property code	Value	Unit	Source
ie	7.00 ± 0.10	eV	NIST Webbook
log10ws	-7.91		Crippen Method
logp	5.146		Crippen Method
mcvol	205.340	ml/mol	McGowan Method

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=C248964&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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