4H-Benzo[def]carbazole

Other names:	Benzo[def]carbazole
	4,5-Iminophenanthrene
	4,5-epiminophenanthrene
Inchi:	InChI=1S/C14H9N/c1-3-9-7-8-10-4-2-6-12-14(10)13(9)11(5-1)15-12/h1-8,15H
InchiKey:	VQOUCGZKKPJLGH-UHFFFAOYSA-N
Formula:	C14H9N
SMILES:	c1cc2ccc3cccc4[nH]c(c1)c2c34
Mol. weight [g/mol]:	191.23
CAS:	203-65-6

Physical Properties

Property code	Value	Unit	Source
ie	7.60 ± 0.10	eV	NIST Webbook
log10ws	-5.52		Crippen Method
logp	3.430		Crippen Method
mcvol	144.560	ml/mol	McGowan Method
rinpol	363.42		NIST Webbook
rinpol	363.92		NIST Webbook
rinpol	364.22		NIST Webbook
rinpol	362.82		NIST Webbook
rinpol	361.90		NIST Webbook
rinpol	361.51		NIST Webbook
rinpol	363.42		NIST Webbook
rinpol	362.82		NIST Webbook
rinpol	362.82		NIST Webbook

Sources

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=C203656&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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