

2,4-Dimethylcarbazole

Inchi:	InChI=1S/C14H13N/c1-9-7-10(2)14-11-5-3-4-6-12(11)15-13(14)8-9/h3-8,15H,1-2H3
InchiKey:	RPSRJMHXZQGERE-UHFFFAOYSA-N
Formula:	C14H13N
SMILES:	Cc1cc(C)c2c(c1)[nH]c1cccc12
Mol. weight [g/mol]:	195.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	3.456		Crippen Method
mcvol	159.720	ml/mol	McGowan Method
rinpol	1932.00		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=U326012&Units=SI

Legend

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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