

Carbazole, 1,5-dimethyl-

Inchi: InChI=1S/C14H13N/c1-9-5-4-8-12-13(9)11-7-3-6-10(2)14(11)15-12/h3-8,15H,1-2H3
InchiKey: DEQROWVQAJBTMI-UHFFFAOYSA-N
Formula: C14H13N
SMILES: Cc1cccc2c1[nH]c1cccc(C)c12
Mol. weight [g/mol]: 195.26
CAS: 51640-60-9

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	2126.00		NIST Webbook
rinpol	2126.00		NIST Webbook

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=C51640609&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

Latest version available from:

<https://www.chemeo.com/cid/12-702-8/Carbazole-1-5-dimethyl.pdf>

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