

Carbazole, 1,4-dimethyl-

Inchi: InChI=1S/C14H13N/c1-9-7-8-10(2)14-13(9)11-5-3-4-6-12(11)15-14/h3-8,15H,1-2H3
InchiKey: APYQRKDHRDGCBK-UHFFFAOYSA-N
Formula: C14H13N
SMILES: Cc1ccc(C)c2c1[nH]c1cccc12
Mol. weight [g/mol]: 195.26
CAS: 18028-55-2

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	1912.00		NIST Webbook
rinpol	343.16		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C18028552&Units=SI>
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>

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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<https://www.chemeo.com/cid/14-612-6/Carbazole-1-4-dimethyl.pdf>

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