

N-methyl-tetrahydrocarbazole

Inchi: InChI=1S/C13H15N/c1-14-12-8-4-2-6-10(12)11-7-3-5-9-13(11)14/h2,4,6,8H,3,5,7,9H2,1H
InchiKey: LXRZSWPAXJBXQM-UHFFFAOYSA-N
Formula: C13H15N
SMILES: Cn1c2c(c3ccccc31)CCCC2
Mol. weight [g/mol]: 185.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.06		Crippen Method
logp	3.057		Crippen Method
mcvol	154.230	ml/mol	McGowan Method
rinpol	1838.00		NIST Webbook
rinpol	1838.00		NIST Webbook
ripol	2651.00		NIST Webbook
ripol	2709.00		NIST Webbook
ripol	2651.00		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=R135127&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/80-024-6/N-methyl-tetrahydrocarbazole.pdf>

Generated by Cheméo on 2024-04-27 08:47:01.535501035 +0000 UTC m=+16496870.456078351.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.