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