N-ethyl-tetrahydrocarbazole

Inchi: InChI=1S/C14H17N/c1-2-15-13-9-5-3-7-11(13)12-8-4-6-10-14(12)15/h3,5,7,9H,2,4,6,8,1
InchiKey: LXUXLQWNCNGZIB-UHFFFAOYSA-N
Formula: C14H17N
SMILES: CCn1c2c(c3ccccc31)CCCC2
Mol. weight [g/mol]: 199.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.04		Crippen Method
logp	3.540		Crippen Method
mcvol	168.320	ml/mol	McGowan Method
rinpol	1857.00		NIST Webbook
rinpol	1857.00		NIST Webbook
ripol	2663.00		NIST Webbook
ripol	2617.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R135112&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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