

N-butyl-tetrahydrocarbazole

Inchi: InChI=1S/C16H21N/c1-2-3-12-17-15-10-6-4-8-13(15)14-9-5-7-11-16(14)17/h4,6,8,10H,2
InchiKey: PCGUZWDQIOEQQC-UHFFFAOYSA-N
Formula: C16H21N
SMILES: CCCCN1c2c(c3ccccc31)CCCC2
Mol. weight [g/mol]: 227.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.87		Crippen Method
logp	4.320		Crippen Method
mcvol	196.500	ml/mol	McGowan Method
rinpol	2016.00		NIST Webbook
rinpol	2016.00		NIST Webbook
ripol	2723.00		NIST Webbook
ripol	2772.00		NIST Webbook
ripol	2723.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R135107&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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