

4-Butylisoquinoline

Inchi:	InChI=1S/C13H15N/c1-2-3-6-11-9-14-10-12-7-4-5-8-13(11)12/h4-5,7-10H,2-3,6H2,1H3
InchiKey:	UTSIRRMCWIVVAR-UHFFFAOYSA-N
Formula:	C13H15N
SMILES:	CCCCc1cncc2ccccc12
Mol. weight [g/mol]:	185.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.68		Crippen Method
logp	3.577		Crippen Method
mcvol	160.790	ml/mol	McGowan Method
rinpol	1705.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R545529&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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