2-METHYLTETRAHYDRO-BETA-CARBOLINE

Other names:	1H-Pyrido[3,4-b]indole, 2,3,4,9-tetrahydro-2-methyl- 2-Methyltetrahydro-b-carboline 2-Methyltetrahydro-«beta»-carboline
Inchi:	InChI=1S/C12H14N2/c1-14-7-6-10-9-4-2-3-5-11(9)13-12(10)8-14/h2-5,13H,6-8H2,1H3
InchiKey:	JOFKCNJIUXPJAC-UHFFFAOYSA-N
Formula:	C12H14N2
SMILES:	CN1CCc2c([nH]c3ccccc23)C1
Mol. weight [g/mol]:	186.26

Physical Properties

Property code	Value	Unit	Source
logp	1.674		Crippen Method
mcvol	150.120	ml/mol	McGowan Method
rinpol	1944.30		NIST Webbook
tb	612.19	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13100000&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature