

# 2-Methyl-1,2,3,4-tetrahydro-«beta»-carboline

<b>Other names:</b>	1H-Pyrido[3,4-b]indole, 2,3,4,9-tetrahydro-2-methyl-2-Methyltetrahydro-b-carboline 2-Methyltetrahydro-«beta»-carboline
<b>Inchi:</b>	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
<b>InchiKey:</b>	JOFKCNJIUXPJAC-UHFFFAOYSA-N
<b>Formula:</b>	C12H14N2
<b>SMILES:</b>	CN1CCc2c([nH]c3cccc23)C1
<b>Mol. weight [g/mol]:</b>	186.25
<b>CAS:</b>	13100-00-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	1.674		Crippen Method
mcvol	150.120	ml/mol	McGowan Method
rropol	1944.30		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13100000&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13100000&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rropol:</b>	Non-polar retention indices

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