

# 1,3-Dimethyl-5-(3-hydroxycyclohexen-1-yl)hexahy

<b>Inchi:</b>	InChI=1S/C12H16N2O4/c1-13-10(16)9(11(17)14(2)12(13)18)7-4-3-5-8(15)6-7/h6,8-9,15
<b>InchiKey:</b>	OFGTVOFOBZROMK-UHFFFAOYSA-N
<b>Formula:</b>	C12H16N2O4
<b>SMILES:</b>	CN1C(=O)C(C2=CC(O)CCC2)C(=O)N(C)C1=O
<b>Mol. weight [g/mol]:</b>	252.27

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.07		Crippen Method
logp	0.124		Crippen Method
mcvol	184.460	ml/mol	McGowan Method
rinpol	2015.00		NIST Webbook
rinpol	2015.00		NIST Webbook

## Sources

<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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R577670&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R577670&amp;Units=SI</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>rinpol:</b>	Non-polar retention indices

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