

# Methohexitone-permethyated

<b>Other names:</b>	Methohexital methyl derivative Methohexital Me
<b>Inchi:</b>	InChI=1S/C15H20N2O3/c1-6-8-9-11(3)15(10-7-2)12(18)16(4)14(20)17(5)13(15)19/h7,11
<b>InchiKey:</b>	VNTOMIJNFGGMEG-UHFFFAOYSA-N
<b>Formula:</b>	C15H20N2O3
<b>SMILES:</b>	C=CCC1(C(C)C#CCC)C(=O)N(C)C(=O)N(C)C1=O
<b>Mol. weight [g/mol]:</b>	276.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Crippen Method
logp	1.649		Crippen Method
mcvol	223.120	ml/mol	McGowan Method
rinpol	1710.00		NIST Webbook
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## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<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=U298732&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U298732&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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