

# Dehydroaphylline

<b>Inchi:</b>	InChI=1S/C15H22N2O/c18-15-12-9-11(13-5-2-4-8-17(13)15)10-16-7-3-1-6-14(12)16/h6,1
<b>InchiKey:</b>	ZNPIGJLCHSRBBI-UHFFFAOYSA-N
<b>Formula:</b>	C15H22N2O
<b>SMILES:</b>	O=C1C2CC(CN3CCCC=C23)C2CCCCN12
<b>Mol. weight [g/mol]:</b>	246.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	1.997		Crippen Method
mcvol	196.000	ml/mol	McGowan Method
rinsol	2190.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R322128&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R322128&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>
<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>

## 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>rinsol:</b>	Non-polar retention indices

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