

# 1,8-Diaza-tricyclo[7.6.0.0\*3,7\*]pentadeca-3(7),8-die

<b>Inchi:</b>	InChI=1S/C13H18N2O/c16-13-10-6-5-7-11(10)14-12-8-3-1-2-4-9-15(12)13/h1-9H2
<b>InchiKey:</b>	IFHZRKSBMOVGFU-UHFFFAOYSA-N
<b>Formula:</b>	C13H18N2O
<b>SMILES:</b>	O=c1c2c(nc3n1CCCCC3)CCC2
<b>Mol. weight [g/mol]:</b>	218.29

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	1.849		Crippen Method
mcvol	174.380	ml/mol	McGowan Method
rinpol	2081.00		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.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=R318317&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R318317&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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