

# Adenine, 1-benzyl-9-cyclopentyl-

<b>Inchi:</b>	InChI=1S/C17H19N5/c18-16-15-17(22(12-19-15)14-8-4-5-9-14)20-11-21(16)10-13-6-2-1
<b>InchiKey:</b>	YSXRHGYTLFNCDZ-UHFFFAOYSA-N
<b>Formula:</b>	C17H19N5
<b>SMILES:</b>	<chem>N=c1c2ncn(C3CCCC3)c2ncn1Cc1ccccc1</chem>
<b>Mol. weight [g/mol]:</b>	293.37

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.73		Crippen Method
logp	2.876		Crippen Method
mcvol	226.750	ml/mol	McGowan Method

## Sources

<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=B6008432&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008432&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>

## 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

Latest version available from:

<https://www.cheméo.com/cid/38-949-7/Adenine-1-benzyl-9-cyclopentyl.pdf>

Generated by Cheméo on 2024-04-23 19:36:12.894978359 +0000 UTC m=+16190221.815555672.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.