

# Adenine, 9-(3,5-o-isopropylidene-beta-d-xylofuranosyl)-

<b>Inchi:</b>	InChI=1S/C13H17N5O4/c1-13(2)20-3-6-9(22-13)8(19)12(21-6)18-5-17-7-10(14)15-4-16-
<b>InchiKey:</b>	XHZOUHXBGRSPRW-UHFFFAOYSA-N
<b>Formula:</b>	C13H17N5O4
<b>SMILES:</b>	CC1(C)OCC2OC(n3cnc4c(N)ncnc43)C(O)C2O1
<b>Mol. weight [g/mol]:</b>	307.31
<b>CAS:</b>	7687-49-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	-0.182		Crippen Method
mcvol	206.770	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7687492&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7687492&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.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>

## 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

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