

# Adenine, 9-butyl-

<b>Inchi:</b>	InChI=1S/C9H13N5/c1-2-3-4-14-6-13-7-8(10)11-5-12-9(7)14/h5-6H,2-4H2,1H3,(H2,10,1
<b>InchiKey:</b>	BKXMJMZKKNYRD-UHFFFAOYSA-N
<b>Formula:</b>	C9H13N5
<b>SMILES:</b>	CCCCn1cnc2c(N)ncnc21
<b>Mol. weight [g/mol]:</b>	191.23
<b>CAS:</b>	2715-70-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	1.209		Crippen Method
mcvol	148.650	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2715700&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2715700&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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