

# Purine, 2-amino-6-ethoxy-

<b>Inchi:</b>	InChI=1S/C7H9N5O/c1-2-13-6-4-5(10-3-9-4)11-7(8)12-6/h3H,2H2,1H3,(H3,8,9,10,11,12)
<b>InchiKey:</b>	SFXXRVSPZSOREJ-UHFFFAOYSA-N
<b>Formula:</b>	C7H9N5O
<b>SMILES:</b>	CCOc1nc(N)nc2nc[nH]c12
<b>Mol. weight [g/mol]:</b>	179.18
<b>CAS:</b>	51866-19-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	-0.148		Crippen Method
mcvol	126.340	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=C51866194&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C51866194&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>

## 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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