

# 2,6(Or 5)-pyrazinediol, 3-amino-5(or 6)-methyl-

<b>Inchi:</b>	InChI=1S/C5H7N3O2/c1-2-4(9)8-5(10)3(6)7-2/h1H3,(H2,6,7)(H2,8,9,10)
<b>InchiKey:</b>	PJDMWYLJWBZCAD-UHFFFAOYSA-N
<b>Formula:</b>	C5H7N3O2
<b>SMILES:</b>	Cc1nc(N)c(=O)[nH]c1O
<b>Mol. weight [g/mol]:</b>	141.13
<b>CAS:</b>	116659-94-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.46		Crippen Method
logp	-1.116		Crippen Method
mcvol	99.230	ml/mol	McGowan Method

## Sources

<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=C116659940&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659940&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>

## 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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