

# 1,6-dimethyl-2(1H)-pyrazinone

<b>Inchi:</b>	InChI=1S/C6H8N2O/c1-5-3-7-4-6(9)8(5)2/h3-4H,1-2H3
<b>InchiKey:</b>	MVOFQFRALBXVIA-UHFFFAOYSA-N
<b>Formula:</b>	C6H8N2O
<b>SMILES:</b>	Cc1cncc(=O)n1C
<b>Mol. weight [g/mol]:</b>	124.14

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	0.089		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
rinpola	1315.00		NIST Webbook

## 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=R221040&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R221040&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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
<b>rinpola:</b>	Non-polar retention indices

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