

# 2(1H)-Pyridinone, 1-methyl-

<b>Other names:</b>	1-Methyl-1,2-dihydro-2-pyridinone 1-Methyl-1H-pyridin-2-one 1-Methyl-2(1H)-pyridinone 1-Methyl-2(1H)-pyridone 1-Methyl-2-oxopyridine 1-Methyl-2-pyridinone 1-Methyl-2-pyridone 1-methylpyridine-2-one 2(1H)-Pyridone, 1-methyl- N-Methyl-2-pyridone N-Methylpyridone NSC 9383
<b>Inchi:</b>	InChI=1S/C6H7NO/c1-7-5-3-2-4-6(7)8/h2-5H,1H3
<b>InchiKey:</b>	DVVGIIUUJYPYENY-UHFFFAOYSA-N
<b>Formula:</b>	C6H7NO
<b>SMILES:</b>	Cn1cccc1=O
<b>Mol. weight [g/mol]:</b>	109.13
<b>CAS:</b>	694-85-9

## Physical Properties

Property code	Value	Unit	Source
affp	925.80	kJ/mol	NIST Webbook
basg	894.80	kJ/mol	NIST Webbook
ie	8.41	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.58 ± 0.02	eV	NIST Webbook
ie	8.41 ± 0.03	eV	NIST Webbook
log10ws	0.96		Aqueous Solubility Prediction Method
logp	0.385		Crippen Method
mcvol	87.490	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	60.20	kJ/mol	376.00	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	523.20	K	98.70	NIST Webbook

## Sources

<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>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</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=C694859&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C694859&amp;Units=SI</a>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<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>tbrp:</b>	Boiling point at reduced pressure

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