

# Pyridine, 4-methyl-, 1-oxide

<b>Other names:</b>	«gamma»-Picoline N-oxide 4-Picoline, 1-oxide «gamma»-Picoline 1-oxide 4-Methylpyridine N-oxide 4-Methylpyridine 1-oxide 4-Picoline N-oxide
<b>Inchi:</b>	InChI=1S/C6H7NO/c1-6-2-4-7(8)5-3-6/h2-5H,1H3
<b>InchiKey:</b>	IWYYIZOHWPCALJ-UHFFFAOYSA-N
<b>Formula:</b>	C6H7NO
<b>SMILES:</b>	Cc1cc[n+](=[O-])cc1
<b>Mol. weight [g/mol]:</b>	109.13
<b>CAS:</b>	1003-67-4

## Physical Properties

Property code	Value	Unit	Source
chs	-3360.90 ± 2.10	kJ/mol	NIST Webbook
hfs	-0.50 ± 2.10	kJ/mol	NIST Webbook
hfs	12.90 ± 0.90	kJ/mol	NIST Webbook
hsub	85.30 ± 2.60	kJ/mol	NIST Webbook
hsub	79.10 ± 1.30	kJ/mol	NIST Webbook
ie	8.17	eV	NIST Webbook
ie	8.12 ± 0.02	eV	NIST Webbook
log10ws	-3.48		Crippen Method
logp	0.628		Crippen Method
mcvol	87.490	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	79.10 ± 1.30	kJ/mol	328.50	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=C1003674&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003674&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>chs:</b>	Standard solid enthalpy of combustion
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation 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

Latest version available from:

<https://www.chemeo.com/cid/29-350-1/Pyridine-4-methyl-1-oxide.pdf>

Generated by Cheméo on 2024-04-10 06:26:38.084417644 +0000 UTC m=+15019647.004994955.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.