

# 3-Pyridinecarboxamide, 1-oxide

<b>Other names:</b>	Nicotinamide, 1-oxide Nicotinamide N-oxide 3-Pyridinecarboxamide N-oxide
<b>Inchi:</b>	InChI=1S/C6H6N2O2/c7-6(9)5-2-1-3-8(10)4-5/h1-4H,(H2,7,9)
<b>InchiKey:</b>	USSFUVKEHXDAPM-UHFFFAOYSA-N
<b>Formula:</b>	C6H6N2O2
<b>SMILES:</b>	NC(=O)c1ccc[n+][[O-]]c1
<b>Mol. weight [g/mol]:</b>	138.12
<b>CAS:</b>	1986-81-8

## Physical Properties

Property code	Value	Unit	Source
hsub	119.20 ± 2.30	kJ/mol	NIST Webbook
log10ws	-3.17		Crippen Method
logp	-0.581		Crippen Method
mvol	99.040	ml/mol	McGowan Method

## 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>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=C1986818&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1986818&amp;Units=SI</a>

## Legend

<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mvol:</b>	McGowan's characteristic volume

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