

# Nicotinonitrile, 2-hydroxy-4-(methoxymethyl)-6-methyl-

<b>Other names:</b>	Pyridine-3-carbonitrile, 1,2-dihydro-4-(methoxymethyl)-6-methyl-2-oxo-4-(Methoxymethyl)-6-methyl-2-oxo-1,2-dihydro-3-pyridinecarbonitrile 3-Cyano-4-methoxymethyl-6-methyl-(2-pyridone) 1,2-Dihydro-4-methoxymethyl-6-methyl-2-oxo-3-pyridinecarbonitrile 3-Pyridinecarbonitrile, 1,2-dihydro-4-(methoxymethyl)-6-methyl-2-oxo-2-Methyl-4-methoxymethyl-5-cyano-6-hydroxypyridine 5-Cyano-6-hydroxy-2-methyl-4-(methoxymethyl)pyridine
<b>Inchi:</b>	InChI=1S/C9H10N2O2/c1-6-3-7(5-13-2)8(4-10)9(12)11-6/h3H,5H2,1-2H3,(H,11,12)
<b>InchiKey:</b>	KLNRUMOPNATILS-UHFFFAOYSA-N
<b>Formula:</b>	C9H10N2O2
<b>SMILES:</b>	<chem>COCc1cc(C)[nH]c(=O)c1C#N</chem>
<b>Mol. weight [g/mol]:</b>	178.19
<b>CAS:</b>	6339-38-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.33		Crippen Method
logp	0.220		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
ss	269.23	J/molxK	NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	211.76	J/molxK	298.15	NIST Webbook

## 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=C6339384&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6339384&amp;Units=SI</a>

## Legend

<b>cps:</b>	Solid phase heat capacity
<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>ss:</b>	Solid phase molar entropy at standard conditions

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