

2(1H)-Pyridinone, 3-methyl-

Other names:	2-Hydroxy-3-methylpyridine 2(1H)-Pyridone, 3-methyl- 3-Methyl-2-pyridinol 3-Methyl-2-pyridone 3-methyl-2(1H)-pyridinone
Inchi:	InChI=1S/C6H7NO/c1-5-3-2-4-7-6(5)8/h2-4H,1H3,(H,7,8)
InchiKey:	MVKDNXIKAWKCCS-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	Cc1ccc[nH]c1=O
Mol. weight [g/mol]:	109.13
CAS:	1003-56-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.59		Crippen Method
logp	0.201		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
ripol	2030.00		NIST Webbook
ripol	2030.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003561&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

ripol: Polar retention indices

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