

2(1H)-Pyridinone, 5-methyl-

Other names:	2(1H)-Pyridone, 5-methyl- 5-Methyl-2-pyridinol 3-Methyl-6-hydroxypyridine 5-methyl-2(1H)-pyridinone 5-methyl-2-pyridone
Inchi:	InChI=1S/C6H7NO/c1-5-2-3-6(8)7-4-5/h2-4H,1H3,(H,7,8)
InchiKey:	SOHMZGMHXUQHGE-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	Cc1ccc(=O)[nH]c1
Mol. weight [g/mol]:	109.13
CAS:	1003-68-5

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	1191.00		NIST Webbook
ripol	2001.00		NIST Webbook
ripol	2001.00		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=C1003685&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

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