

2(1H)-Pyridone, 6-methyl-

Other names:	6-Methyl-2-pyridinol 2(1H)-Pyridinone, 6-methyl- 2-Methyl-6-pyridone 6-Methyl-2-hydroxypyridine 6-Methyl-2-pyridinone 6-Methyl-2-pyridone 2-Hydroxy-6-methylpyridine 6-Methyl-2-pyridyl alcohol 6-Methyl-2(1H)-pyridone 2-Methyl-6-hydroxypyridine 6-Methyl-2(1H)-pyridinone 6-methylpyridin-2-ol
Inchi:	InChI=1S/C6H7NO/c1-5-3-2-4-6(8)7-5/h2-4H,1H3,(H,7,8)
InchiKey:	JEAVIRYCMBDJIU-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	<chem>Cc1cccc(=O)[nH]1</chem>
Mol. weight [g/mol]:	109.13
CAS:	3279-76-3

Physical Properties

Property code	Value	Unit	Source
chs	-3149.20 ± 1.90	kJ/mol	NIST Webbook
hf	-120.30 ± 2.50	kJ/mol	NIST Webbook
hfs	-212.30 ± 2.10	kJ/mol	NIST Webbook
hsub	92.00 ± 1.30	kJ/mol	NIST Webbook
hsub	92.00 ± 1.30	kJ/mol	NIST Webbook
ie	8.19 ± 0.03	eV	NIST Webbook
log10ws	-0.59		Crippen Method
logp	0.201		Crippen Method
mcvol	87.490	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3279763&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hsub: Enthalpy of sublimation at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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