

# 6-Methyluracil

<b>Other names:</b>	2(1H)-Pyrimidinone, 4-hydroxy-6-methyl- 2,4(1H,3H)-Pyrimidinedione, 6-methyl- 2,4-Dihydroxy-6-methylpyrimidine 2,4-Pyrimidinediol, 6-methyl- 4-(6)-Methyluracil 4-Methyluracil 6-Methyl-1H-pyrimidine-2,4-dione AWD 23-15 NSC 9456 Pseudothymine Uracil, 6-methyl-
<b>Inchi:</b>	InChI=1S/C5H6N2O2/c1-3-2-4(8)7-5(9)6-3/h2H,1H3,(H2,6,7,8,9)
<b>InchiKey:</b>	SHVCSCWHWMSGTE-UHFFFAOYSA-N
<b>Formula:</b>	C5H6N2O2
<b>SMILES:</b>	<chem>Cc1cc(=O)[nH]c(=O)[nH]1</chem>
<b>Mol. weight [g/mol]:</b>	126.11
<b>CAS:</b>	626-48-2

## Physical Properties

Property code	Value	Unit	Source
chs	-2356.90 ± 0.25	kJ/mol	NIST Webbook
chs	-2374.00	kJ/mol	NIST Webbook
chs	-2372.70	kJ/mol	NIST Webbook
hsub	131.00	kJ/mol	NIST Webbook
log10ws	-1.26		Aqueous Solubility Prediction Method
logp	-1.592		Crippen Method
mcvol	89.250	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cps	162.50	J/mol×K	298.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	167.20	J/mol×K	303.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	170.20	J/mol×K	308.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	172.20	J/mol×K	313.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	176.90	J/mol×K	318.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	181.40	J/mol×K	323.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	183.00	J/mol×K	328.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	187.30	J/mol×K	333.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	190.40	J/mol×K	338.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	193.00	J/mol×K	343.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

## Sources

Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry: McGowan Method:	<a href="https://www.doi.org/10.1021/je060257y">https://www.doi.org/10.1021/je060257y</a>
Aqueous Solubility Prediction Method:	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a>
	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C626482&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C626482&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Thermochemical study of 5-methyluracil, 6-methyluracil, and 5-nitrouracil:	<a href="https://www.doi.org/10.1016/j.jct.2011.06.023">https://www.doi.org/10.1016/j.jct.2011.06.023</a>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>cps:</b>	Solid phase heat capacity
<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>mcvol:</b>	McGowan's characteristic volume

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