6-Methyluracil

Other names:	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-
Inchi:	InChI=1S/C5H6N2O2/c1-3-2-4(8)7-5(9)6-3/h2H,1H3,(H2,6,7,8,9)
InchiKey:	SHVCSCWHWMSGTE-UHFFFAOYSA-N
Formula:	C5H6N2O2
SMILES:	Cc1cc(=O)[nH]c(=O)[nH]1
Mol. weight [g/mol]:	126.11
CAS:	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

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:	https://www.doi.org/10.1021/je060257y
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C626482&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermochemical study of 5-methyluracil, 6-methyluracil, and 5-nitrouracil:	https://www.doi.org/10.1016/j.jct.2011.06.023

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume