6-METHYLURACIL

Other names:	2(1H)-Pyrimidinone, 4-hydroxy-6-methyl-
	2,4(1H,3H)-Pyrimidinedione, 6-methyl-
	2,4-Pyrimidinediol, 6-methyl-
	2,4-dihydroxy-6-methylpyrimidine
	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

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
tf	491.33	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Thermochemical study of 5-methyluracil, 6-methyluracil, and 5-nitrouracil:	https://www.doi.org/10.1016/j.jct.2011.06.023
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C626482&Units=SI

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

tf: Normal melting (fusion) point