Thymine

Other names:	1-methyl-2,4(1H,3H)-pyrimidinedione 1-methyluracil 2,4(1H,3H)-Pyrimidinedione, 5-methyl- 2,4(1H,3H)-pyrimidinedione, 1-methyl- 2,4-Dihydroxy-5-methylpyrimidine 5-Methyl-2,4(1H,3H)-pyrimidinedione 5-Methyl-2,4-dioxypyrimidine 5-Methyluracil 5-methyl-2,4-dihydroxypyrimidine 5-methylpyrimidine-2,4(1H,3H)-dione N1-methyluracil Thymin
Inchi:	InChI=1S/C5H6N2O2/c1-3-2-6-5(9)7-4(3)8/h2H,1H3,(H2,6,7,8,9)
InchiKey:	RWQNBRDOKXIBIV-UHFFFAOYSA-N
Formula:	C5H6N2O2
SMILES:	Cc1c[nH]c(=O)[nH]c1=O
Mol. weight [g/mol]:	126.11
CAS:	65-71-4

Physical Properties

Property code	Value	Unit	Source
affp	880.90	kJ/mol	NIST Webbook
basg	850.00	kJ/mol	NIST Webbook
chl	-2362.23 ± 0.84	kJ/mol	NIST Webbook
chs	-2367.30	kJ/mol	NIST Webbook
chs	-2369.00	kJ/mol	NIST Webbook
ea	0.07 ± 0.01	eV	NIST Webbook
ea	0.07 ± 0.02	eV	NIST Webbook
ea	0.06 ± 0.01	eV	NIST Webbook
ea	0.07	eV	NIST Webbook
ea	2.40 ± 0.10	eV	NIST Webbook
hf	-328.70 ± 4.30	kJ/mol	NIST Webbook
hfl	-462.80 ± 0.84	kJ/mol	NIST Webbook
hsub	134.10 ± 4.20	kJ/mol	NIST Webbook
hsub	138.00 ± 10.00	kJ/mol	NIST Webbook
hsub	131.30 ± 4.00	kJ/mol	NIST Webbook
hvap	134.10 ± 4.20	kJ/mol	NIST Webbook

ie	9.40 ± 0.10	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.00 ± 0.10	eV	NIST Webbook
ie	9.02	eV	NIST Webbook
ie	9.14 ± 0.03	eV	NIST Webbook
log10ws	-1.51		Estimated Solubility Method
log10ws	-1.55		Aqueous Solubility Prediction Method
logp	-1.592		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
tf	321.30 ± 1.00	K	NIST Webbook
tf	589.53	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	223.00	J/mol×K	328.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	179.60	J/mol×K	308.15	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	156.90	J/mol×K	298.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	211.10	J/mol×K	323.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	151.40	J/mol×K	298.15	NIST Webbook
cps	150.20	J/mol×K	298.00	NIST Webbook
cps	256.10	J/mol×K	343.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	245.90	J/mol×K	338.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	235.00	J/mol×K	333.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	200.50	J/mol×K	318.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	190.90	J/mol×K	313.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
hfust	17.51	kJ/mol	321.30	NIST Webbook
hfust	17.51	kJ/mol	321.30	NIST Webbook
hfust	17.51	kJ/mol	321.30	NIST Webbook
hsubt	125.70 ± 3.60	kJ/mol	410.50	NIST Webbook
hsubt	124.40 ± 1.30	kJ/mol	403.00	NIST Webbook
psub	3.97e-03	kPa	450.80	Thermochemistry of uracil and thymine revisited
psub	0.02	kPa	472.30	Thermochemistry of uracil and thymine revisited
psub	0.01	kPa	468.90	Thermochemistry of uracil and thymine revisited
psub	0.01	kPa	464.80	Thermochemistry of uracil and thymine revisited
psub	8.13e-03	kPa	460.60	Thermochemistry of uracil and thymine revisited
psub	6.01e-03	kPa	456.50	Thermochemistry of uracil and thymine revisited
psub	3.14e-03	kPa	447.60	Thermochemistry of uracil and thymine revisited
psub	1.83e-03	kPa	440.50	Thermochemistry of uracil and thymine revisited
psub	1.34e-03	kPa	436.20	Thermochemistry of uracil and thymine revisited
psub	8.60e-04	kPa	430.50	Thermochemistry of uracil and thymine revisited
psub	6.10e-04	kPa	426.40	Thermochemistry of uracil and thymine revisited

rhos	1450.00	kg/m3	298.15	Saturation molalities and standard molar enthalpies of solution of cytidine(cr), hypoxanthine(cr), thymidine(cr), thymine(cr), uridine(cr), and xanthine(cr) in H2O(l)

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Thermochemical study of 5-methyluracil, 6-methyluracil, and 5-nitrouracil:	https://www.doi.org/10.1016/j.jct.2011.06.023
Solvation behavior of some nucleic acid bases and nucleosides in water and in aqueous guanidine hydrochloride solutions: Volumetric, calorimetric and spectroscopic	https://www.doi.org/10.1016/j.jct.2015.11.029
Heat Capacities of Uracil, Thymine, and Its Alkylated Cyclooligomethylenated, Adamantylated Derivatives by Differential Calorimetry:	https://www.doi.org/10.1021/je060257y
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65714&Units=SI
Saturation molalities and standard molar enthalpies of solution of cytidine(cr), hypoxanthine(cr), thymidine(cr), thymine(cr), uridine(cr), and xanthine(cr) in H2O(l):	https://www.doi.org/10.1016/j.jct.2004.04.005
Thermochemistry of uracil and thymine revisited:	https://www.doi.org/10.1016/j.jct.2015.03.015
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Volumetric studies on nucleic acid bases and nucleosides in aqueous guanidine hydrochloride solutions at T = (288.15 to 318.15) K and at atmospheric pressure:	https://www.doi.org/10.1016/j.jct.2014.10.015

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
psub:	Sublimation pressure
rhos:	Solid Density
tf:	Normal melting (fusion) point