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

InChl=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	0.06 ± 0.01	eV	NIST Webbook
ea	2.40 ± 0.10	eV	NIST Webbook
ea	0.07 ± 0.02	eV	NIST Webbook
ea	0.07 ± 0.01	eV	NIST Webbook
ea	0.07	eV	NIST Webbook
hf	-328.70 ± 4.30	kJ/mol	NIST Webbook
hfl	-462.80 ± 0.84	kJ/mol	NIST Webbook
hsub	138.00 ± 10.00	kJ/mol	NIST Webbook
hsub	134.10 ± 4.20	kJ/mol	NIST Webbook
hsub	131.30 ± 4.00	kJ/mol	NIST Webbook
hvap	134.10 ± 4.20	kJ/mol	NIST Webbook

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

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source	
cps	223.00	J/mol×K	328.15 Cyd	Heat Capacities of Uracil, Thymine, and Its Alkylated, clooligomethylenate and Halogenated Derivatives by Differential Calorimetry	ed,
cps	179.60	J/mol×K	308.15 Cyd	Heat Capacities of Uracil, Thymine, and Its Alkylated, clooligomethylenate and Halogenated Derivatives by Differential Calorimetry	ed,
cps	167.20	J/mol×K	303.15 Cyd	Heat Capacities of Uracil, Thymine, and Its Alkylated, clooligomethylenate and Halogenated Derivatives by Differential Calorimetry	ed,

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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C65714&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l Solvation behavior of some nucleic https://www.doi.org/10.1016/j.jct.2015.11.029

https://www.doi.org/10.1016/j.jct.2014.10.015

http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

bouvation behavior of some nucleic acid bases and nucleosides in water should be a solution behavior of some nucleic acid bases and nucleosides in water should be a solution of the state https://www.doi.org/10.1016/j.jct.2011.06.023 https://www.doi.org/10.1016/j.jct.2004.04.005 molar enthalpies of solution of the molar enthalpies of the molar

Legend

affp: Proton affinity basg: Gas basicity

chl: Standard liquid enthalpy of combustion chs: Standard solid enthalpy of combustion

Solid phase heat capacity cps:

Electron affinity ea:

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/llogp:Octanol/Water partition coefficientmcvol:McGowan's characteristic volume

psub: Sublimation pressure

rhos: Solid Density

tf: Normal melting (fusion) point

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