

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	0.06 ± 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/molxK	328.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	179.60	J/molxK	308.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	167.20	J/molxK	303.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	156.90	J/molxK	298.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	211.10	J/molxK	323.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	151.40	J/molxK	298.15	NIST Webbook
cps	150.20	J/molxK	298.00	NIST Webbook
cps	256.10	J/molxK	343.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	245.90	J/molxK	338.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	235.00	J/molxK	333.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	200.50	J/molxK	318.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	190.90	J/molxK	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

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

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