2,4(1H,3H)-Pyrimidinedione, 5-methyl-

Other names:	2,4-dihydroxy-5-methylpyrimidine
	5-Methyl-2,4(1H,3H)-pyrimidinedione
	5-Methyl-2,4-dioxypyrimidine
	5-methyl-2,4-dihydroxypyrimidine
	5-methylpyrimidine-2,4(1H,3H)-dione
	5-methyluracil
	Thymin
	thymine
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

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	-2369.00	kJ/mol	NIST Webbook
chs	-2367.30	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	9.00 ± 0.10	eV	NIST Webbook
ie	9.14 ± 0.03	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.02	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	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	150.20	J/mol×K	298.00	NIST Webbook
cps	151.40	J/mol×K	298.15	NIST Webbook
cps	189.90	J/mol×K	323.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	205.90	J/mol×K	343.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	184.30	J/mol×K	318.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	200.00	J/mol×K	333.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	195.20	J/mol×K	328.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	178.70	J/mol×K	313.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	203.50	J/mol×K	338.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	173.70	J/mol×K	308.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	168.20	J/mol×K	303.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	163.00	J/mol×K	298.15	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	8.13e-03	kPa	460.60	Thermochemistry of uracil and thymine revisited
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	6.10e-04	kPa	426.40	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	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	0.01	kPa	464.80	Thermochemistry of uracil and thymine revisited
psub	8.60e-04	kPa	430.50	Thermochemistry of uracil and thymine revisited
psub	0.01	kPa	468.90	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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry:	https://www.doi.org/10.1021/je060257y
Saturation molalities and standard molar enthalpies of solution of cytidine(cr), hypoxanthine(cr), thymidine(cr), uracil(cr), uridine(cr), and xanthine(cr) in H2O(l):	https://www.doi.org/10.1016/j.jct.2004.04.005
Solvation behavior of some nucleic acid bases and nucleosides in water, dimethylsulfoxide, and their binary mixtures:	https://www.doi.org/10.1016/j.jct.2015.11.029
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Thermochemical study of 5-methyluracil, 6-methyluracil, and 5-nitrouracil:	https://www.doi.org/10.1016/j.jct.2011.06.023
Thermochemistry of uracil and thymine revisited:	https://www.doi.org/10.1016/j.jct.2015.03.015
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65714&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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