Uracil

Other names:	1H-Pyrimidine-2,4-dione
	2,4(1H,3H)-Pyrimidinedione
	2,4-Dihydroxypyrimidine
	2,4-Dioxopyrimidine
	2,4-Dioxypyrimidine
	2,4-Pyrimidinediol
	2,4-Pyrimidinedione
	2,6-Dihydroxypyrimidine
	2-Hydroxy-4(1H)-pyrimidinone
	2-Hydroxy-4(3H)-pyrimidinone
	4-Hydroxy-2(1H)-pyrimidinone
	Hybar X
	NSC 3970
	Pirod
	Pyrod
	RU 12709
	Ura
Inchi:	InChI=1S/C4H4N2O2/c7-3-1-2-5-4(8)6-3/h1-2H,(H2,5,6,7,8)
InchiKey:	ISAKRJDGNUQOIC-UHFFFAOYSA-N
Formula:	C4H4N2O2
SMILES:	O=c1cc[nH]c(=O)[nH]1
Mol. weight [g/mol]:	112.09
CAS:	66-22-8

Physical Properties

Property code	Value	Unit	Source
affp	872.70	kJ/mol	NIST Webbook
affp	858.00	kJ/mol	NIST Webbook
basg	841.70	kJ/mol	NIST Webbook
chs	-1716.14 ± 0.28	kJ/mol	NIST Webbook
chs	-1721.30 ± 2.20	kJ/mol	NIST Webbook
ea	0.08	eV	NIST Webbook
ea	0.09 ± 0.01	eV	NIST Webbook
ea	2.49 ± 0.10	eV	NIST Webbook
ea	0.05 ± 0.04	eV	NIST Webbook
ea	0.09 ± 0.01	eV	NIST Webbook
hf	-303.10 ± 2.30	kJ/mol	NIST Webbook

hfs	-429.56 ± 0.60	kJ/mol	NIST Webbook
hfs	-424.40 ± 2.50	kJ/mol	NIST Webbook
hsub	131.00 ± 5.00	kJ/mol	NIST Webbook
hsub	126.50 ± 2.20	kJ/mol	NIST Webbook
hsub	84.00	kJ/mol	NIST Webbook
ie	9.59	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	9.45	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.40 ± 0.10	eV	NIST Webbook
ie	9.53 ± 0.02	eV	NIST Webbook
ie	9.80 ± 0.10	eV	NIST Webbook
ie	9.68	eV	NIST Webbook
ie	9.50 ± 0.03	eV	NIST Webbook
log10ws	-1.49		Estimated Solubility Method
log10ws	-1.61		Aqueous Solubility Prediction Method
logp	-1.901		Crippen Method
mcvol	75.160	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	131.80	J/mol×K	298.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	151.80	J/mol×K	328.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	149.00	J/mol×K	323.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	146.10	J/mol×K	318.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	143.00	J/mol×K	313.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	140.90	J/mol×K	308.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	135.50	J/mol×K	303.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	120.50	J/mol×K	298.00	NIST Webbook
cps	157.40	J/mol×K	343.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	156.80	J/mol×K	338.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	154.30	J/mol×K	333.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
hsubt	125.30 ± 0.20	kJ/mol	375.00	NIST Webbook
hsubt	101.30	kJ/mol	405.00	NIST Webbook
hsubt	127.00 ± 2.00	kJ/mol	444.00	NIST Webbook
hsubt	130.60 ± 4.00	kJ/mol	519.50	NIST Webbook
hsubt	120.50 ± 1.30	kJ/mol	403.00	NIST Webbook
hsubt	121.70	kJ/mol	425.00	NIST Webbook
hsubt	120.50 ± 5.20	kJ/mol	425.50	NIST Webbook
hsubt	126.50 ± 2.20	kJ/mol	440.00	NIST Webbook
hsubt	134.00 ± 8.00	kJ/mol	522.50	NIST Webbook
psub	2.20e-04	kPa	424.00	Thermochemistry of uracil and thymine revisited
psub	5.10e-04	kPa	434.10	Thermochemistry of uracil and thymine revisited
psub	1.35e-03	kPa	446.00	Thermochemistry of uracil and thymine revisited
psub	2.12e-03	kPa	451.90	Thermochemistry of uracil and thymine revisited
psub	3.17e-03	kPa	457.70	Thermochemistry of uracil and thymine revisited
psub	4.70e-03	kPa	462.60	Thermochemistry of uracil and thymine revisited
psub	6.73e-03	kPa	467.40	Thermochemistry of uracil and thymine revisited
psub	8.60e-04	kPa	440.00	Thermochemistry of uracil and thymine revisited
psub	9.05e-03	kPa	472.40	Thermochemistry of uracil and thymine revisited

rhol	1070.30	kg/m3	343.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1073.30	kg/m3	338.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1076.20	kg/m3	333.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1079.30	kg/m3	328.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1082.30	kg/m3	323.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1085.30	kg/m3	318.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1088.40	kg/m3	313.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis

rhol	1091.40	kg/m3	308.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1094.50	kg/m3	303.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis
rhol	1097.60	kg/m3	298.15	Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
Solvation behavior of some nucleic acid bases and nucleosides in water	https://www.doi.org/10.1016/j.jct.2015.11.029
McGowan Method: Guanidine hydrochloride solutions: Viscometric, calorimetric and spectroscopic approach:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66228&Units=SI
Solubilities in Water of Uracil and Its Halogenated Derivatives:	https://www.doi.org/10.1021/je800029c
Thermochemistry of uracil and thymine revisited:	https://www.doi.org/10.1016/j.jct.2015.03.015
Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry:	https://www.doi.org/10.1021/je060257y
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Measurement and Correlation of Solubility of Uracil in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je800614u
Nucleic acid bases in 1-alkyl-3-methylimidazolium acetate ionic liquids: A thermophysical and ionic conductivity analysis:	https://www.doi.org/10.1016/j.jct.2012.07.022
Volumetric and transport properties of betaine hydrochloride ions in aqueous uracil solutions at T = (298.15-318.15) K:	https://www.doi.org/10.1016/j.jct.2016.03.008
Thermodynamic Investigation of Uracil and Its Halo Derivatives. Enthalpies of Solution and Solvation in Methanol:	https://www.doi.org/10.1021/je049656o
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
psub:	Sublimation pressure
rhol:	Liquid Density

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