

5-Iodouracil

Other names:	2,4(1H,3H)-Pyrimidinedione, 5-iodo- 2,4-dihydroxy-5-iodopyrimidine 5-iodo-2,4-pyrimidinedione NSC 57848 Uracil, 5-iodo- pyrimidine, 2,4-dihydroxy-5-iodo-
Inchi:	InChI=1S/C4H3IN2O2/c5-2-1-6-4(9)7-3(2)8/h1H,(H2,6,7,8,9)
InchiKey:	KSNXJLQDQOIRIP-UHFFFAOYSA-N
Formula:	C4H3IN2O2
SMILES:	O=c1[nH]cc(I)c(=O)[nH]1
Mol. weight [g/mol]:	237.98
CAS:	696-07-1

Physical Properties

Property code	Value	Unit	Source
log10ws	0.10		Crippen Method
logp	-1.296		Crippen Method
mcvol	100.980	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	150.90	J/mol×K	298.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	153.90	J/mol×K	303.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	156.80	J/mol×K	308.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	159.80	J/mol×K	313.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	162.80	J/mol×K	318.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	165.80	J/mol×K	323.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	168.60	J/mol×K	328.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	170.30	J/mol×K	333.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	172.70	J/molxK	338.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	177.50	J/molxK	343.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
hsubt	127.00	kJ/mol	386.50	NIST Webbook

Sources

Thermodynamic Investigation of Uracil and Its Halo Derivatives. Enthalpies of Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry: McGowan Method:	https://www.doi.org/10.1021/je049656o
Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry:	https://www.doi.org/10.1021/je060257y
Solubilities in Water of Uracil and Its Halogenated Derivatives:	https://www.doi.org/10.1021/je800029c
Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C696071&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cps:	Solid phase heat capacity
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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