

2,4(1H,3H)-Pyrimidinedione, 1,3-dimethyl-

Other names:	1,3-dimethyl-2,4-(1H,3H)-pyrimidinedione 1,3-dimethyluracil 2,4-Dihydroxy-1,3-dimethylpyrimidine N,N'-Dimethyluracil N1,N3-Dimethyluracil Uracil, 1,3-dimethyl-
Inchi:	InChI=1S/C6H8N2O2/c1-7-4-3-5(9)8(2)6(7)10/h3-4H,1-2H3
InchiKey:	JSDBKAHWADVXFU-UHFFFAOYSA-N
Formula:	C6H8N2O2
SMILES:	Cn1ccc(=O)n(C)c1=O
Mol. weight [g/mol]:	140.14
CAS:	874-14-6

Physical Properties

Property code	Value	Unit	Source
chs	-3093.87 ± 0.29	kJ/mol	NIST Webbook
ea	0.04 ± 0.10	eV	NIST Webbook
hf	-313.60 ± 1.50	kJ/mol	NIST Webbook
hfs	-410.50 ± 0.90	kJ/mol	NIST Webbook
hsub	96.90 ± 1.20	kJ/mol	NIST Webbook
hsub	96.40 ± 1.40	kJ/mol	NIST Webbook
hsub	92.00	kJ/mol	NIST Webbook
hvap	71.00 ± 3.00	kJ/mol	NIST Webbook
ie	8.80 ± 0.10	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-2.89		Crippen Method
logp	-0.916		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
tf	392.50 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	170.00	J/mol×K	298.15	NIST Webbook

cps	185.40	J/mol×K	303.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	188.70	J/mol×K	308.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	191.20	J/mol×K	313.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	193.80	J/mol×K	318.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	196.40	J/mol×K	323.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	199.10	J/mol×K	328.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	201.00	J/mol×K	333.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	203.30	J/mol×K	338.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	206.80	J/mol×K	343.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	182.50	J/mol×K	298.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
hfust	23.10	kJ/mol	392.50	NIST Webbook
hfust	14.60	kJ/mol	398.00	NIST Webbook
hfust	14.60	kJ/mol	398.00	NIST Webbook
hsubt	96.90	kJ/mol	298.15	NIST Webbook
hsubt	115.80 ± 3.00	kJ/mol	339.00	NIST Webbook
hsubt	101.70 ± 2.10	kJ/mol	338.00	NIST Webbook
hsubt	46.00 ± 4.20	kJ/mol	427.00	NIST Webbook
hsubt	92.00	kJ/mol	357.00	NIST Webbook
psub	7.73e-05	kPa	308.20	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	7.41e-04	kPa	327.80	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	2.47e-04	kPa	318.00	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	1.99e-03	kPa	337.60	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil

psub	2.17e-05	kPa	298.30	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	1.42e-03	kPa	334.90	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	5.27e-04	kPa	324.80	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	1.76e-04	kPa	315.00	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	6.46e-05	kPa	306.60	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	1.09e-03	kPa	331.80	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	3.95e-04	kPa	321.90	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	1.24e-04	kPa	312.10	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	3.65e-05	kPa	302.20	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	1.09e-05	kPa	293.30	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	0.02	kPa	360.50	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	4.90e-03	kPa	347.80	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil

psub	1.86e-03	kPa	338.00	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	9.03e-03	kPa	354.70	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	3.60e-03	kPa	344.90	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	1.32e-03	kPa	335.10	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	6.69e-03	kPa	351.70	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	2.64e-03	kPa	341.90	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
psub	0.01	kPa	357.70	Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil
sfust	58.90	J/mol×K	392.50	NIST Webbook
ssubt	325.00	J/mol×K	298.15	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Hydrogenated Derivatives by Crippen Method: <https://www.doi.org/10.1021/je060257y>

Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil: <https://www.doi.org/10.1021/je500719p>

Crippen Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C874146&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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
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
sfust:	Entropy of fusion at a given temperature
ssubt:	Entropy of sublimation at a given temperature
tf:	Normal melting (fusion) point

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