2,4(1H,3H)-Pyrimidinedione, 1,3,6-trimethyl-

Other names:	1,3,4-trimethyluracil
	1,3,6-trimethyl-2,4(1H,3H)-pyrimidinedione
	1,3,6-trimethyluracil
	Uracil, 1,3,6-trimethyl-
Inchi:	InChI=1S/C7H10N2O2/c1-5-4-6(10)9(3)7(11)8(5)2/h4H,1-3H3
InchiKey:	GRDXZRWCQWDLPG-UHFFFAOYSA-N
Formula:	C7H10N2O2
SMILES:	Cc1cc(=O)n(C)c(=O)n1C
Mol. weight [g/mol]:	154.17
CAS:	13509-52-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	-0.608		Crippen Method
mcvol	117.430	ml/mol	McGowan Method
tf	384.50 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	236.50	J/mol×K	338.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	239.60	J/mol×K	343.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	212.60	J/mol×K	298.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	213.50	J/mol×K	303.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	217.10	J/mol×K	308.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	218.50	J/mol×K	313.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	219.80	J/mol×K	318.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	223.40	J/mol×K	323.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	228.30	J/mol×K	328.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	229.00	J/mol×K	333.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
hfust	21.20	kJ/mol	384.50	NIST Webbook
hfust	21.20	kJ/mol	384.50	NIST Webbook
hfust	21.20	kJ/mol	384.50	NIST Webbook
hsubt	106.70 ± 2.50	kJ/mol	320.00	NIST Webbook
sfust	55.10	J/mol×K	384.50	NIST Webbook

Sources

Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry:	https://www.doi.org/10.1021/je060257y
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13509529&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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tf:	Normal melting (fusion) point