1,3-Dimethyl-5-ethyluracil

Other names:	2,4(1H,3H)-pyrimidinedione, 5-ethyl-1,3-dimethyl- uracil, 5-ethyl-1,3-dimethyl-
Inchi:	InChI=1S/C8H12N2O2/c1-4-6-5-9(2)8(12)10(3)7(6)11/h5H,4H2,1-3H3
InchiKey:	RGFNQXKFHSVDHI-UHFFFAOYSA-N
Formula:	C8H12N2O2
SMILES:	CCc1cn(C)c(=O)n(C)c1=O
Mol. weight [g/mol]:	168.19
CAS:	31703-08-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	-0.354		Crippen Method
mcvol	131.520	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	291.10	J/mol×K	343.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	281.70	J/mol×K	338.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	275.20	J/mol×K	333.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	270.70	J/mol×K	328.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	241.10	J/mol×K	298.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	250.10	J/mol×K	303.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	256.50	J/mol×K	308.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	261.00	J/mol×K	313.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
cps	264.30	J/mol×K	318.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry

cps	267.40	J/mol×K	323.15	Heat Capacities of Uracil, Thymine, and Its Alkylated, Cyclooligomethylenated, and Halogenated Derivatives by Differential Calorimetry
hfust	19.40	kJ/mol	354.40	NIST Webbook
hsubt	110.00 ± 1.20	kJ/mol	329.50	NIST Webbook
hsubt	99.30 ± 0.20	kJ/mol	308.00	NIST Webbook
hsubt	98.70 ± 1.70	kJ/mol	316.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31703089&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

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