6-AMINO-1,3-DIMETHYLURACIL

Other names:	1,3-Dimethyl-6-amino-uracil
	2,4(1H,3H)-Pyrimidinedione, 6-amino-1,3-dimethyl-
	4-Amino-1,3-dimethyl-2,6-dihydroxypyrimidine
	4-Amino-1,3-dimethyluracil
	Uracil, 6-amino-1,3-dimethyl-
Inchi:	InChI=1S/C6H9N3O2/c1-8-4(7)3-5(10)9(2)6(8)11/h3H,7H2,1-2H3
InchiKey:	VFGRNTYELNYSKJ-UHFFFAOYSA-N
Formula:	C6H9N3O2
SMILES:	Cn1c(N)cc(=O)n(C)c1=O
Mol. weight [g/mol]:	155.16

Physical Properties

Property code	Value	Unit	Source
hf	-324.25	kJ/mol	Cheméo Relay (1.0)
logp	-1.334		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
tb	591.20	K	Cheméo Relay (1.0)
tf	484.49	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	189.00	J/mol×K	298.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	208.00	J/mol×K	343.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry

cps	206.00	J/mol×K	338.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	204.00	J/mol×K	333.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	201.60	J/mol×K	328.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	199.50	J/mol×K	323.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	197.30	J/mol×K	318.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	195.20	J/mol×K	313.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	193.10	J/mol×K	308.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	191.00	J/mol×K	303.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
psub	2.87e-05	kPa	412.67	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil

psub	1.05e-04	kPa	425.66	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil	
psub	6.08e-05	kPa	420.22	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil	
psub	5.34e-05	kPa	418.41	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil	
psub	3.97e-05	kPa	416.43	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil	
psub	4.48e-05	kPa	415.86	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil	
psub	3.13e-05	kPa	412.82	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil	

psub	9.90e-06	kPa	401.59	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	2.48e-05	kPa	410.80	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	2.31e-05	kPa	409.99	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	1.85e-05	kPa	409.00	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	1.67e-05	kPa	407.21	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil

Sources

Cheméo Relay (1.0):

Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil:	https://www.doi.org/10.1021/je020215j
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Experimental study on the thermochemistry of some amino derivatives of uracil:	https://www.doi.org/10.1016/j.jct.2011.06.003
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6642315&Units=SI
Cheméo Relay (1.0, beta):	
Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry:	https://www.doi.org/10.1021/je6005168
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point