2,4(1H,3H)-Pyrimidinedione, 5-amino-

Other names:	2,4-Dihydroxy-5-aminopyrimidine
	5-Amino-2,4-dihydroxypyrimidine
	5-amino-2,4(1H,3H)-pyrimidinedione
	5-aminouracil
	Uracil, 5-amino-
Inchi:	InChI=1S/C4H5N3O2/c5-2-1-6-4(9)7-3(2)8/h1H,5H2,(H2,6,7,8,9)
InchiKey:	BISHACNKZIBDFM-UHFFFAOYSA-N
Formula:	C4H5N3O2
SMILES:	Nc1c[nH]c(=O)[nH]c1=O
Mol. weight [g/mol]:	127.10
CAS:	932-52-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.61		Crippen Method
logp	-2.318		Crippen Method
mcvol	85.140	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	151.30	J/mol×K	343.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	150.60	J/mol×K	338.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	150.00	J/mol×K	333.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry

cps	149.10	J/mol×K	328.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	148.40	J/mol×K	323.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	148.00	J/mol×K	318.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	147.00	J/mol×K	313.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	146.20	J/mol×K	308.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	145.50	J/mol×K	303.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	145.00	J/mol×K	298.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
psub	9.97e-05	kPa	453.10	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	6.66e-05	kPa	447.76	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil

psub	5.71e-05	kPa	445.97	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	6.02e-05	kPa	445.96	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	5.37e-05	kPa	445.07	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	5.23e-05	kPa	444.14	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	4.79e-05	kPa	442.32	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	3.89e-05	kPa	440.48	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil

psub	3.33e-05	kPa	438.65	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	2.56e-05	kPa	436.70	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	2.07e-05	kPa	433.16	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil
psub	1.94e-05	kPa	433.11	Vapour pressures, molar enthalpies of sublimation, and molar enthalpies of solution in water of selected amino derivatives of uracil and 5-nitrouracil

Sources

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
Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry:	https://www.doi.org/10.1021/je6005168
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C932525&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

cps:	Solid phase heat capacity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
psub:	Sublimation pressure