

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	145.00	J/molxK	298.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	145.50	J/molxK	303.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry
cps	146.20	J/molxK	308.15	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	148.00	J/mol×K	318.15	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	149.10	J/mol×K	328.15	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	150.60	J/mol×K	338.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry	
cps	151.30	J/mol×K	343.15	Molar Heat Capacities of Aminouracils by Differential Scanning Calorimetry	
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	

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	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	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	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	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	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	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	5.71e-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	6.66e-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	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

Sources

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. 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/10.1016/j.jct.2011.06.003>

Molar Heat Capacities of Aminoacils by Differential Scanning Calorimetry. <https://www.doi.org/10.1021/je020215j>

McGowan Method: <https://www.doi.org/10.1021/je6005168>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C932525&Units=SI>

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

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