Cytosine

Other names:	2(1H)-Pyrimidinone, 4-amino- 4-Amino-2(1H)-pyrimidinone 4-Amino-2(1H)pyrimidone 4-Amino-2-hydroxypyrimidine 4-Amino-2-oxypyrimidine Cyt Cytosinimine
Inchi:	InChI=1S/C4H5N3O/c5-3-1-2-6-4(8)7-3/h1-2H,(H3,5,6,7,8)
InchiKey:	OPTASPLRGRRNAP-UHFFFAOYSA-N
Formula:	C4H5N3O
SMILES:	Nc1ccnc(=O)[nH]1
Mol. weight [g/mol]:	111.10
CAS:	71-30-7

Physical Properties

Property code	Value	Unit	Source
affp	949.90	kJ/mol	NIST Webbook
basg	918.00	kJ/mol	NIST Webbook
chs	-2053.18 ± 0.37	kJ/mol	NIST Webbook
chs	-2067.30 ± 2.00	kJ/mol	NIST Webbook
ea	0.23 ± 0.01	eV	NIST Webbook
ea	2.34 ± 0.10	eV	NIST Webbook
ea	0.09 ± 0.01	eV	NIST Webbook
hf	-59.00 ± 10.00	kJ/mol	NIST Webbook
hfs	-235.43 ± 0.46	kJ/mol	NIST Webbook
hfs	-221.30 ± 2.30	kJ/mol	NIST Webbook
hsub	167.00 ± 10.00	kJ/mol	NIST Webbook
hsub	176.00 ± 10.00	kJ/mol	NIST Webbook
hsub	176.00 ± 10.00	kJ/mol	NIST Webbook
hsub	155.00 ± 3.00	kJ/mol	NIST Webbook
ie	8.90 ± 0.20	eV	NIST Webbook
ie	8.94 ± 0.03	eV	NIST Webbook
ie	8.45	eV	NIST Webbook
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-1.16		Estimated Solubility Method

log10ws	-1.17		Aqueous Solubility Prediction Method
log10ws	-1.16		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-1.130		Crippen Method
mcvol	79.270	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	132.60	J/mol×K	298.00	NIST Webbook
hsubt	167.70 ± 0.50	kJ/mol	365.00	NIST Webbook
hsubt	151.70 ± 0.70	kJ/mol	515.00	NIST Webbook
hsubt	147.20 ± 2.60	kJ/mol	453.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71307&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

Legend

affp: Proton affinity

basg: Gas basicity

chs: Standard solid enthalpy of combustion

cps: Solid phase heat capacity

ea: Electron affinity

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

hsub: Enthalpy of sublimation at standard conditions

hsubt: Enthalpy of sublimation at a given temperature

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume