Histidine

Other names:	(S)-.alpha.-amino-1H-imidazole-4-propanoic acid
	(S)-4-(2-amino-2-carboxyethyl)imidazole
	(S)-histidine
	1H-Imidazole-4-propanoic acid, «alpha»-amino-, (S)-
	1H-Imidazole-4-propanoic acid, Â«alphaÂ»-amino-, (S)-
	4-(2-Amino-2-carboxyethyl)imidazole
	Anti-rheuma
	D-histidine
	Glyoxaline-5-alanine
	Histidine, L-
	L-(-)-Histidine
	L-Histidine
Inchi:	InChI=1S/C6H9N3O2/c7-5(6(10)11)1-4-2-8-3-9-4/h2-3,5H,1,7H2,(H,8,9)(H,10,11)/t5-/m1
InchiKey:	HNDVDQJCIGZPNO-RXMQYKEDSA-N
Formula:	C6H9N3O2
SMILES:	NC(Cc1c[nH]cn1)C(=O)O
Mol. weight [g/mol]:	155.15
CAS:	71-00-1

Physical Properties

Property code	Value	Unit	Source
affp	979.10	kJ/mol	NIST Webbook
affp	988.40 ± 5.40	kJ/mol	NIST Webbook
affp	996.00 ± 2.80	kJ/mol	NIST Webbook
affp	988.00	kJ/mol	NIST Webbook
basg	941.10 ± 5.40	kJ/mol	NIST Webbook
basg	952.60 ± 3.20	kJ/mol	NIST Webbook
basg	950.20	kJ/mol	NIST Webbook
chs	-3180.60 ± 2.30	kJ/mol	NIST Webbook
chs	-3205.50 ± 2.50	kJ/mol	NIST Webbook
ep	-37.00 ± 5.00	J/mol×K	NIST Webbook
hfs	-466.70 ± 2.80	kJ/mol	NIST Webbook
hfs	-441.80 ± 2.60	kJ/mol	NIST Webbook
log10ws	-0.53		Aqueous Solubility Prediction Method
logp	-1.118		Crippen Method
mcvol	113.320	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	142.00 ± 8.00	kJ/mol	442.00	NIST Webbook

Sources

Volumetric, ultrasonic, and viscometric behaviour of l-histidine in aqueous-glucose solutions at different temperatures:	https://www.doi.org/10.1016/j.jct.2010.11.017
Synthesis and Physical and Thermodynamic Properties of Lactic Acid and Malic Acid-Based Natural Deep Eutectic Solvents:	https://www.doi.org/10.1021/acs.jced.7b01037
Solubility of the Proteinogenic a-Amino Acids in Water, Ethanol, and Ethanol-Water Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00486
Volumetric Behaviour and Interactions of a-Amino Acids with Sodium Acetate, Potassium Acetate, and Calcium Acetate in Aqueous Solutions:	https://www.doi.org/10.1021/je100190e
Interactions in (L-phenylalanine/L-histidine + 0.01 mol kg-1 aqueous beta-cyclodextrin) systems at T = (293.15, 298.15, 303.15 and 308.15) K:	https://www.doi.org/10.1016/j.jct.2012.03.029
Intermolecular Interactions of L-glutamine and L-histidine in Aqueous Solutions of Metformin hydrochloride: Volumetric, Compressibility and Viscometric Studies:	https://www.doi.org/10.1021/acs.jced.5b00549
Partial molar volumes of L-alanine, DL-serine, DL-threonine, L-histidine, glycine, and glycylglycine in water, NaCl, and DMSO aqueous solutions at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2005.03.015
Determining and Modeling of L-Histidine Solubility in Several Pure Solvents from 293.15 to 333.15 K:	https://www.doi.org/10.1021/acs.jced.9b00659
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71001&Units=SI
Surface tension and UV-visible investigations of aggregation and adsorption behavior of NaC and NaDC in water-amino acid mixtures:	https://www.doi.org/10.1016/j.fluid.2015.03.012
Viscosity Behavior of alpha-Amino Acids in Acetate Salt Solutions at Temperatures (303.15 to 323.15) K:	https://www.doi.org/10.1007/s10765-011-1111-y
Modeling solubility and acid-base properties of some polar side chain amino acids in NaCl and (CH3)4NCl aqueous solutions at different ionic strengths and temperatures:	https://www.doi.org/10.1016/j.fluid.2017.11.030
Solubility of L-histidine in different aqueous binary solvent mixtures from 283.15 K to 318.15 K with experimental measurement and thermodynamic modelling:	https://www.doi.org/10.1016/j.jct.2016.09.039
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
APPARENT MOLAR VOLUME, COMPRESSIBILITY AND VISCOMETRIC STUDIES OF SODIUM DODECYL BENZENE SULFONATE (SDBS) AND DODECYLTRIMETHYLAMMONIUM BROMIDE (DTAB) IN AQUEOUS AMINO ACID SOLUTIONS: A THERMO-ACOUSTIC APPROACH:	https://www.doi.org/10.1016/j.tca.2013.12.021
Temperature of Maximum Density for Binary Aqueous Solutions of Five Amino Acids:	https://www.doi.org/10.1021/acs.jced.9b00752
Effect of temperature and additives on the critical micelle concentration and thermodynamics of micelle formation of sodium dodecyl benzene sulfonate and dodecyltrimethylammonium bromide in aqueous solution: A conductometric study:	https://www.doi.org/10.1016/j.jct.2013.12.019
Conductivity and fluorescence studies on the micellization properties of sodium cholate and sodium deoxycholate in aqueous medium at different temperatures: Effect of selected amino acids:	https://www.doi.org/10.1016/j.jct.2014.10.014
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Structure making behaviour of L-histidine in aqueous solutions of ampicillin sodium at different temperatures: Using physicochemical methods:	https://www.doi.org/10.1016/j.jct.2017.07.040
Volumetric, compressibility and viscometric studies on sodium cholate/sodium deoxycholate amino acid interactions in aqueous medium:	https://www.doi.org/10.1016/j.tca.2015.02.014
Ultrasonic Velocities and Densities of L-Histidine or L-Glutamic Acid or l-Tryptophan or Glycylglycine + 2 mol*L-1 Aqueous KCl or KNO3 Solutions from (298.15 to 323.15) K:	https://www.doi.org/10.1021/je900199j
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Viscosities of L-Histidine/L-Glutamic Acid/L-Tryptophan/Glycylglycine+2 M Aqueous KCl/KNO3 Solutions at T =(298.15 to 323.15)K:	https://www.doi.org/10.1007/s10765-011-0996-9

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
ep:	Protonation entropy at 298K
hfs:	Solid phase enthalpy of formation at standard conditions
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