Betaine

Other names:	(carboxymethyl)trimethylammonium hydroxide inner salt (trimethylammonio)acetate 1-Carboxy-N,N,N-trimethylmethanaminium hydroxide, inner salt 2-(Trimethylammonio)ethanoic acid, hydroxide, inner salt Abromine Cystadane Glycine betaine Glycine, trimethylbetaine Glycocoll betaine Glycylbetaine Loramine AMB-13 Lycine Methanaminium, 1-carboxy-N,N,N-trimethyl-, hydroxide, inner salt Methanaminium, 1-carboxy-N,N,N-trimethyl-, inner salt Oxyneurine Rubrine C Trimethylaminoacetate Trimethylaminoacetic acid Trimethylglycine Trimethylglycocoll «alpha»-Earleine
Inchi:	InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
InchiKey:	KWIUHFFTVRNATP-UHFFFAOYSA-N
Formula:	C5H11NO2
SMILES:	C[N+](C)(C)CC(=O)[O-]
Mol. weight [g/mol]:	117.15
CAS:	107-43-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.24		Crippen Method
logp	-1.557		Crippen Method
mcvol	98.730	ml/mol	McGowan Method

Sources

The hydration of the protein stabilizing agents: Trimethylamine-N-oxide, glycine and its N-methylderivatives. The volumetric and compressibility studies:	https://www.doi.org/10.1016/j.jct.2013.01.023
Thermophysical Properties and Solubility of Different Sugar-Derived Molecules in Deep Eutectic Solvents:	https://www.doi.org/10.1021/acs.jced.7b00184
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107437&Units=SI
Compatible solutes: Thermodynamic properties relevant for effective protection against osmotic stress:	https://www.doi.org/10.1016/j.fluid.2015.07.004
Counteracting effects of trimethylamine N-oxide and betaine on the interactions of urea with zwitterionic glycine peptides:	https://www.doi.org/10.1016/j.tca.2009.02.017
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Physical properties of seven deep eutectic solvents based on L-proline or betaine:	https://www.doi.org/10.1016/j.jct.2018.12.017
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
Ternary phase behavior of phenol + toluene + zwitterionic alkaloids for separating phenols from oil mixtures via forming deep eutectic solvents:	https://www.doi.org/10.1016/j.fluid.2017.05.001
Volumetric and calorimetric investigations of molecular interactions in some amino acids and peptides in the combined presence of surfactants and glycine betaine:	https://www.doi.org/10.1016/j.jct.2012.05.031
Partial molar volume and partial molar isentropic compressibility study of glycine betaine in aqueous and aqueous KCl or MgCl2 solutions at temperatures T = 288.15-318.15 K:	https://www.doi.org/10.1016/j.tca.2013.08.002
Modulation of molecular interactions of homologous series of amino acids with sorbitol-glycine betaine mixture compared to individual osmolytes: Thermodynamic analysis:	https://www.doi.org/10.1016/j.jct.2019.05.016
Specific Heat Capacities of Two Functional Ionic Liquids and Two Functional Deep Eutectic Solvents for the Absorption of SO2:	https://www.doi.org/10.1021/acs.jced.7b00102
Mode of action of betaine on some amino acids and globular proteins: Thermodynamic considerations:	https://www.doi.org/10.1016/j.jct.2017.03.025
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility and Solution Thermodynamics of Betaine in Different Pure Solvents and Binary Mixtures:	https://www.doi.org/10.1021/je2011659
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Characterization of the volumetric properties of betaine in aqueous solutions: Compositional, pressure, and temperature dependence:	https://www.doi.org/10.1016/j.tca.2014.03.042

Legend

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