

# 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 Glycocol 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 Trimethylglycocol «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
mccvol	98.730	ml/mol	McGowan Method

# Sources

The hydration of the protein stabilizing agents: Trimethylamine-N-oxide, glycerol and betaine derivatives  
Properties of betaine in aqueous solutions: Compositional, pressure, and temperature dependence: Crippen Method:

<https://www.doi.org/10.1016/j.jct.2013.01.023>  
<https://www.doi.org/10.1016/j.tca.2014.03.042>  
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C107437&Units=SI>  
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Modulation of molecular interactions of homologous series of amino acids with ionic liquids and ionic liquids mixture  
Thermodynamic and molecular interactions of betaine derivatives in the combined presence of two ionic liquids  
Thermodynamic Properties of Sugars in Aqueous and Organic Solvents for the Purification of Alkaloids for Separating the Caffeine from some amino acids and molecular proteins: Thermodynamic Considerations: Solubility of Different Sugar-Derived Nucleosides in Poly Ethanol Solvents: Thermodynamic Properties of Lactic Acid and Malic Acid-Based Natural Deep Eutectic Solvents: Counteracting effects of trimethylamine N-oxide and betaine on the solubility and stability of zwitterionic betaine  
Thermodynamic Properties of Betaine in Different Pure Solvents and Binary Mixtures: Compatible solutes: Thermodynamic properties relevant for effective partial molar volume and partial molar isentropic compressibility study of physical betaine derivatives and deep eutectic solvent based on l-proline or betaine  
Temperatures T = 288.15 318.15 K:

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<https://www.doi.org/10.1016/j.jct.2012.05.031>  
<https://www.doi.org/10.1021/acs.jced.7b00102>  
<https://www.doi.org/10.1016/j.fluid.2017.05.001>  
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<https://www.doi.org/10.1016/j.tca.2009.02.017>  
<https://www.doi.org/10.1021/je2011659>  
<http://link.springer.com/article/10.1007/BF02311772>  
<https://www.doi.org/10.1016/j.fluid.2015.07.004>  
<https://www.doi.org/10.1016/j.tca.2013.08.002>  
<https://www.doi.org/10.1016/j.jct.2018.12.017>

## Legend

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

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