>>**Entry Name: Betaine**
Synonym(s): Carboxy-*N,N,N*-trimethylmethanaminium hydroxide inner salt, 9CI. (Carboxymethyl)trimethylammonium. Glycine betaine. Glycocoll betaine. Lycine. Abromine. Pluchine. Oxyneurine

CAS Registry Number: 107-43-7
Related CAS Registry Numbers(s): 590-47-6

$Me_3N^{(+)}CH_2COO^{(-)}$

Molecular Formula: $C_5H_{11}NO_2$
Molecular Weight: 117.147
Accurate Mass: 117.078979
Percentage Composition: C 51.26%; H 9.46%; N 11.96%; O 27.31%
Biological Source: Prod. by *Aspergillus oryzae, Patella vulgata, Claviceps purpurea* and other fungi. Occurs widely in plants and animals. Alkaloid from *Abroma augusta* (Sterculiaceae)
Use/Importance: May play a part in cytoplasmic osmoregulation. Causes myoatrophy in combination with Guanidinoacetic acid CVS98-F
Physical Description: Deliquescent scales or cryst.; cryst. + $1H_2O$ (H_2O)
pKa Value: pK_a 3.84 (free acid)
Other Data: Dec. at ca. 310° (293-4°) with isom. to Me_2NCH_2COOMe
Hazard & Toxicity: LD_{50} (mus, scu) 10800 mg/kg

Aldrich: 21906-1
Fluka: 14290
Rare Chemicals Library: S39806-3
Sigma: B5648

>>**Derivative:** Monohydrate
Synonym(s): Trimethylglycine hydroxide. Pluchine

CAS Registry Number: 17146-86-0
Use/Importance: Lipotropic
Physical Description: Cryst.
Other Data: Loses water at 100° to form inner salt
Fluka: 14300

>>**Derivative:** Hydrochloride
Synonym(s): Betaine hydrochloride, USAN. Acidol. Lycine hydrochloride. Achylin. Acidin. Acinorm. Acipepsol. Aciventral forte. Euacid. Muriat. Pepsacid

CAS Registry Number: 590-46-5
Use/Importance: Used in solders, fluxes and in org. synth. Lipotropic. Electrolyte replenisher, gastric acidifier
Physical Description: Needles
Melting Point: Mp 243-244 dec.°
Optical Rotation: $[\alpha]_D^{20}$ –29.51 (H_2O)

Aldrich: 14793-1
Fluka: 14295
Rare Chemicals Library: S91431-2
Sigma: B3501

>>**Derivative:** Aspartate (1:1)
Synonym(s): Hepastyl. Somabet. Somatyl

CAS Registry Number: 52921-08-1
Use/Importance: Used in treatment of liver and stomach disorders

>>**Derivative:** Picrate

Physical Description: Yellow prisms (H_2O)
Melting Point: Mp 181-182°

>>**Derivative:** Chloride
see 2-Chloro-*N,N,N*-trimethyl-2-oxoethanaminium(1+), DGN71-D

References: