



>>Entry Name: 3-Amino-1-propanesulfonic acid, 9Cl

Synonym(s): Homotaurine‡

CAS Registry Number: 3687-18-1

Related CAS Registry Numbers(s): 14650-46-5 81028-90-2

$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{SO}_2\text{OH}$

Molecular Formula: $\text{C}_3\text{H}_9\text{NO}_3\text{S}$

Molecular Weight: 139.175

Accurate Mass: 139.030314

Percentage Composition: C 25.89%; H 6.52%; N 10.06%; O 34.49%; S 23.04%

Source/Synthesis: Constit. of marine red algae e.g. *Grateloupia livida*

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 290-292 dec.° (270-271°)

pKa Value: $\text{p}K_{\text{a}}$ 10.05 (H_2O)

Aldrich: A7610-9

Sigma: A5037

>>Derivative: Amide

Molecular Formula: $\text{C}_3\text{H}_{10}\text{N}_2\text{O}_2\text{S}$

Molecular Weight: 138.19

Accurate Mass: 138.046298

Percentage Composition: C 26.07%; H 7.29%; N 20.27%; O 23.16%; S 23.20%

Physical Description: Cryst.

Melting Point: Mp 159-160°

>>Derivative: N-Ac

Synonym(s): 3-Acetylamino-1-propanesulfonic acid, 9Cl. **Acamprosate**, BAN, INN. Aotal. Campral

CAS Registry Number: 77337-76-9

Molecular Formula: $\text{C}_5\text{H}_{11}\text{NO}_4\text{S}$

Molecular Weight: 181.212

Accurate Mass: 181.040879

Percentage Composition: C 33.14%; H 6.12%; N 7.73%; O 35.32%; S 17.70%

Use/Importance: GABA receptor agonist. Psychotropic agent. Used in treatment of alcoholism

Physical Description: Solid (AcOH)

Melting Point: Mp 187-189°

>>Derivative: N-Ac, Ca salt (2:1)

Synonym(s): Calcium N-acetylhomotaurine. Ca-AOTA

CAS Registry Number: 77337-73-6

Melting Point: Mp 270°

Other Data: Na, K, Li, Mg and Zn salts also reported

>>Derivative: N-Benzoyl

Molecular Formula: $\text{C}_{10}\text{H}_{13}\text{NO}_4\text{S}$

Molecular Weight: 243.283

Accurate Mass: 243.056529

Percentage Composition: C 49.37%; H 5.39%; N 5.76%; O 26.31%; S 13.18%

Physical Description: Cryst. (EtOH aq.) (as Ag salt)

>>Derivative: N-Me

Molecular Formula: $\text{C}_4\text{H}_{11}\text{NO}_3\text{S}$

Molecular Weight: 153.202

Accurate Mass: 153.045964

Percentage Composition: C 31.36%; H 7.24%; N 9.14%; O 31.33%; S 20.93%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 210-212°

References: