



>>Entry Name: 2-Aminoethanesulfonic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Taurine, 8CI, INN. Aminoethylsulfonic acid. Ethylaminesulfonic acid

CAS Registry Number: 107-35-7

Related CAS Registry Numbers(s): 4316-74-9 7347-25-3

$\text{H}_2\text{NCH}_2\text{CH}_2\text{SO}_3\text{H}$

Molecular Formula:  $\text{C}_2\text{H}_7\text{NO}_3\text{S}$

Molecular Weight: 125.148

Accurate Mass: 125.014664

Percentage Composition: C 19.19%; H 5.64%; N 11.19%; O 38.35%; S 25.62%

Use/Importance: Intermed. in metab. of cysteine. Used as an adjunct in treatment of hypercholesterolaemia. Metabolic regulator

Physical Description: Monoclinic prismatic rods

Melting Point: Mp 328° (320-325° dec.)

Solubility: Sol.  $\text{H}_2\text{O}$ , insol. EtOH; BERDY SOL: Sol.  $\text{H}_2\text{O}$

pKa Value:  $\text{p}K_{\text{a}1}$  1.5;  $\text{p}K_{\text{a}2}$  8.74

Other Data: Dec. ca. 300°

Hazard & Toxicity: LD<sub>50</sub> (mus, scu) 6 g/kg

Aldrich: W38130-6

Fluka: 86330

Sigma: T9931

>>Derivative: Amide

CAS Registry Number: 4378-70-5

Molecular Formula:  $\text{C}_2\text{H}_8\text{N}_2\text{O}_2\text{S}$

Molecular Weight: 124.163

Accurate Mass: 124.030648

Percentage Composition: C 19.35%; H 6.49%; N 22.56%; O 25.77%; S 25.83%

Physical Description: Plates (EtOH) (as hydrochloride)

Melting Point: Mp 133° (hydrochloride)

>>Derivative: N-Me

CAS Registry Number: 107-68-6

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%

Biological Source: Isol. from red algae *Ptilota pectinata* and others

Physical Description: Prisms

Melting Point: Mp 241-242°

Solubility: V. sol.  $\text{H}_2\text{O}$ , insol. EtOH, Et<sub>2</sub>O

Rare Chemicals Library: S56095-2

>>Derivative: N,N-Di-Me

CAS Registry Number: 637-95-6

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%

Biological Source: Obt. from *Corallina officinalis*. Present in red algae

Physical Description: Prisms (MeOH)

Melting Point: Mp 315-316 dec.°

Solubility: V. sol.  $\text{H}_2\text{O}$ , AcOH, insol. EtOH, Et<sub>2</sub>O