



>>Entry Name: (3-Aminopropyl)(carboxymethyl)dimethylammonium betaine

Synonym(s): 3-Amino-*N*-(carboxymethyl)-*N,N*-dimethyl-1-propanaminium hydroxide inner salt, 9Cl

CAS Registry Number: 36574-66-0

Related CAS Registry Numbers(s): 52504-27-5 61789-40-0

Extra CAS Registry Numbers(s): 60114-62-7

$\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{N}^{(+)}\text{Me}_2\text{CH}_2\text{COO}^{(-)}$

Molecular Formula: $\text{C}_7\text{H}_{16}\text{N}_2\text{O}_2$

Molecular Weight: 160.216

Accurate Mass: 160.121178

Percentage Composition: C 52.48%; H 10.07%; N 17.48%; O 19.97%

General Statement: Zwitterionic

Other Data: In addition to the individual acyl homologues listed as derivatives, a nonstoichiometric mixture of homologues, Cocamidopropyl betaine or Cocamidopropyldimethylglycine derived from coconut oil fatty acids, has similar uses in shampoos, liquid hand soaps, etc.

>>Derivative: *N*-Dodecanoyl

Synonym(s): *N*-(Carboxymethyl)-*N,N*-dimethyl-3-[(1-oxododecyl)amino]-1-propanaminium hydroxide inner salt, 9Cl. (Carboxymethyl)(3-lauramidopropyl)dimethylammonium hydroxide inner salt, 8Cl

CAS Registry Number: 4292-10-8

Molecular Formula: $\text{C}_{19}\text{H}_{38}\text{N}_2\text{O}_3$

Molecular Weight: 342.521

Accurate Mass: 342.288243

Percentage Composition: C 66.63%; H 11.18%; N 8.18%; O 14.01%

Use/Importance: Surfactant used in cosmetics

Physical Description: Soft wax

>>Derivative: *N*-Hexadecanoyl

Synonym(s): *N*-(Carboxymethyl)-*N,N*-dimethyl-3-[(1-oxohexadecyl)amino]-1-propanaminium hydroxide inner salt. (Carboxymethyl)dimethyl(3-palmitamidopropyl)ammonium hydroxide inner salt. **Pentadecamaine**, BAN, INN. Tegobetaine

CAS Registry Number: 32954-43-1

Molecular Formula: $\text{C}_{23}\text{H}_{46}\text{N}_2\text{O}_3$

Molecular Weight: 398.628

Accurate Mass: 398.350843

Percentage Composition: C 69.30%; H 11.63%; N 7.03%; O 12.04%

Use/Importance: Surface-active agent used in surgical scrubs

References:

U.S. Pat., 1965, 32205074; *CA*, **64**, 17431g, (*synth*)

Ger. Pat., 1971, *Hough Hoseason*, 2 060 439; *CA*, **75**, 50725, (*use*)

Eur. Pat., 1982, 20907; *CA*, **94**, 174298j, (*synth*)

Hart, J.R., *Drug Cosmet. Ind.*, 1984, **134**, 46; 48; 50, (*use*)

Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **22**, 322, (*use*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1215