



>>Entry Name: Benzylhexadecyldimethylammonium(1+)

Synonym(s): *N*-Hexadecyl-*N,N*-dimethylbenzenemethanaminium, 9Cl. Cetalkonium. Acinol. Armil. Baktonium. Banicol. Bicetonium. Ceetolan. Cetol. Spilan. Tetraseptan. Zettyn. NSC 32942. Win 357



Molecular Formula: C₂₅H₄₆N⁽⁺⁾

Molecular Weight: 360.645

Accurate Mass: 360.363024

Percentage Composition: C 83.26%; H 12.86%; N 3.88%

Use/Importance: Antiinfective and surface-active agent

Physical Description: Cryst. (EtOAc/petrol)

>>Derivative: Chloride

Synonym(s): Cetalkonium chloride, BAN, INN, USAN

CAS Registry Number: 122-18-9

Molecular Formula: C₂₅H₄₆ClN

Molecular Weight: 396.098

Accurate Mass: 395.331876

Percentage Composition: C 75.81%; H 11.71%; Cl 8.95%; N 3.54%

Melting Point: Mp 68° (59°)

Aldrich: 22900-8

Fluka: 13400

Rare Chemicals Library: S56065-0

Sigma: B4136

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 673C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1321C, (*ir*)

U.S. Pat., 1937, 2 075 958; *CA*, **31**, 3597, (*synth, props*)

Westphal, O. *et al.*, *Ber.*, 1940, **73**, 1011, (*synth*)

Shelton, R.S. *et al.*, *J.A.C.S.*, 1946, **68**, 753, (*synth, props*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 787