

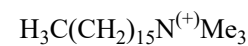


>>Entry Name: Hexadecyltrimethylammonium(1+), 8Cl

Synonym(s): *N,N,N*-Trimethyl-1-hexadecanaminium, 9Cl. Cetyltrimethylammonium. Cetrimonium

CAS Registry Number: 6899-10-1

Related CAS Registry Numbers(s): 505-86-2 8044-71-1



Molecular Formula: $\text{C}_{19}\text{H}_{42}\text{N}^{(+)}$

Molecular Weight: 284.547

Accurate Mass: 284.331724

Percentage Composition: C 80.20%; H 14.88%; N 4.92%

Use/Importance: Topical antiseptic, preservative, surfactant. Reagent for isol. and purifn. of acidic polysaccharides and sulfonated carbohydrates. Used as 0.2-0.3% aq. soln. Increases sensitivity in photometric detn. of metals (e.g. Al, Be, In, Th, Zr) with some chelating reagents (e.g. chromazurol S, bromopyrogallol red, phenylfluorone); forms ternary complexes

>>Derivative: Chloride

Synonym(s): Cetrimonium chloride, BAN. Aliquat 6. Variquat E228. CETAC

CAS Registry Number: 112-02-7

Molecular Formula: $\text{C}_{19}\text{H}_{42}\text{ClN}$

Molecular Weight: 320

Accurate Mass: 319.300576

Percentage Composition: C 71.32%; H 13.23%; Cl 11.08%; N 4.38%

Aldrich: 29273-7

Fluka: 52366

>>Derivative: Bromide

Synonym(s): Cetrimonium bromide, INN. Cetab. Cirrasol OD. Many other names

CAS Registry Number: 57-09-0

Molecular Formula: $\text{C}_{19}\text{H}_{42}\text{BrN}$

Molecular Weight: 364.451

Accurate Mass: 363.27006

Percentage Composition: C 62.62%; H 11.62%; Br 21.92%; N 3.84%

Physical Description: Microcryst.

Melting Point: Mp 237-243°

Solubility: Sol. H_2O , EtOH; insol. C_6H_6 , Et_2O

Other Data: Component of Cetrimide, BAN

Hazard & Toxicity: LD₅₀ (rat, orl) 410 mg/kg. Exp. reprod. and teratogenic effects

Aldrich: 85582-0

Fluka: 52370

Sigma: C9252

>>Derivative: Pentachlorophenolate

Synonym(s): TCAP. T.S.P.

CAS Registry Number: 87-76-3

Molecular Formula: $\text{C}_{25}\text{H}_{42}\text{Cl}_5\text{NO}$

Molecular Weight: 549.876

Accurate Mass: 547.170899

Percentage Composition: C 54.61%; H 7.70%; Cl 32.24%; N 2.55%; O 2.91%

Use/Importance: Topical antiseptic, fungicide

>>Derivative: 4-Methylbenzenesulfonate

Synonym(s): Cetrimonium tosylate. Intol

CAS Registry Number: 138-32-9

Molecular Formula: $\text{C}_{26}\text{H}_{49}\text{NO}_3\text{S}$

Molecular Weight: 455.744

Accurate Mass: 455.343314

Percentage Composition: C 68.52%; H 10.84%; N 3.07%; O 10.53%; S 7.04%

Fluka: 52436

Sigma: C8147