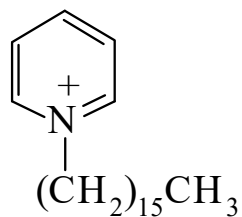




>>Entry Name: 1-Hexadecylpyridinium(1+)

Synonym(s): Cetylpyridinium. Ceepryn. Many other names



CAS Registry Number: 7773-52-6

Related CAS Registry Numbers(s): 6004-24-6

Molecular Formula: $C_{21}H_{38}N^{(+)}$

Molecular Weight: 304.538

Accurate Mass: 304.300424

Percentage Composition: C 82.82%; H 12.58%; N 4.60%

Use/Importance: Surface active agent with bactericidal properties; used in throat pastilles etc. Used as a 0.2-0.3% aq. soln. to increase sensitivity in photometric detn. of metals; forms ternary complexes with metal ions and some chromogenic reagents

Calculated Log P Data: Log P 5.24 (uncertain value) (calc)

>>Derivative: Chloride

Synonym(s): Cetylpyridinium chloride, BAN, INN. Biosept. Ceepryn. Cepacol. Cephim. Cetafilm. Merocet

CAS Registry Number: 123-03-5

Molecular Formula: $C_{21}H_{38}ClN$

Molecular Weight: 339.991

Accurate Mass: 339.269276

Percentage Composition: C 74.19%; H 11.27%; Cl 10.43%; N 4.12%

Melting Point: Mp 87-88°

Solubility: Sol. H_2O

Other Data: Monohydrate, Mp 77-83°

Hazard & Toxicity: Eye and skin irritant. LD₅₀ (rat, orl) 200 mg/kg

>>Derivative: Bromide

Synonym(s): Acetoquat CPB. Bromocet. Cetapharm. Cetasol. Cetazol 80. Nitrogenol. Sterogenol

CAS Registry Number: 140-72-7

Molecular Formula: $C_{21}H_{38}BrN$

Molecular Weight: 384.442

Accurate Mass: 383.23876

Percentage Composition: C 65.61%; H 9.96%; Br 20.78%; N 3.64%

Physical Description: Microcryst.

Melting Point: Mp 61-62°. Mp 66-68°

Solubility: Sol. H_2O , EtOH

Fluka: 52340

Rare Chemicals Library: S51968-5

Sigma: C5881

>>Derivative: Iodide

CAS Registry Number: 2349-55-5

Molecular Formula: $C_{21}H_{38}IN$

Molecular Weight: 431.442

Accurate Mass: 431.204897

Percentage Composition: C 58.46%; H 8.88%; I 29.41%; N 3.25%

Melting Point: Mp 101°

References: