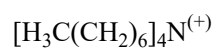




>>Entry Name: Tetraheptylammonium(1+)

Synonym(s): *N,N,N*-Triheptylheptanaminium(1+), 9Cl

CAS Registry Number: 35414-25-6



Molecular Formula: $\text{C}_{28}\text{H}_{60}\text{N}^{(+)}$

Molecular Weight: 410.789

Accurate Mass: 410.472574

Percentage Composition: C 81.87%; H 14.72%; N 3.41%

>>Derivative: Hydroxide

Molecular Formula: $\text{C}_{28}\text{H}_{61}\text{NO}$

Molecular Weight: 427.796

Accurate Mass: 427.475314

Percentage Composition: C 78.61%; H 14.37%; N 3.27%; O 3.74%

Use/Importance: Reagent for on-column heptylation of barbiturates for gc sepn.

Other Data: Prepd. in MeOH soln. from the iodide

>>Derivative: Chloride

CAS Registry Number: 10247-90-2

Molecular Formula: $\text{C}_{28}\text{H}_{60}\text{ClN}$

Molecular Weight: 446.241

Accurate Mass: 445.441426

Percentage Composition: C 75.36%; H 13.55%; Cl 7.94%; N 3.14%

Physical Description: Yellow liq.

Melting Point: Mp -9°

Density: d_{35} 0.8817

Aldrich: 41990-7

Fluka: 87292

>>Derivative: Bromide

CAS Registry Number: 4368-51-8

Molecular Formula: $\text{C}_{28}\text{H}_{60}\text{BrN}$

Molecular Weight: 490.693

Accurate Mass: 489.41091

Percentage Composition: C 68.54%; H 12.32%; Br 16.28%; N 2.85%

Use/Importance: Used for prep. of liq. membranes for anion selective electrodes; used in chromatographic sepn. of steroids. Commercially available. Ion-pair agent used in sepn. of org. acids by ion-pair reversed-phase tlc

Physical Description: Hygroscopic flaky powder

Melting Point: Mp $87-89^\circ$

Hazard & Toxicity: Irritant

Aldrich: 39693-1

Fluka: 87296

Sigma: T6533

>>Derivative: Iodide

CAS Registry Number: 3535-83-9

Molecular Formula: $\text{C}_{28}\text{H}_{60}\text{IN}$

Molecular Weight: 537.693

Accurate Mass: 537.377047

Percentage Composition: C 62.55%; H 11.25%; I 23.60%; N 2.60%

Melting Point: Mp $121-122^\circ$

Fluka: 87288

Other: PB T04630

>>Derivative: Carbonate (1:2)

CAS Registry Number: 42485-81-4

Use/Importance: Used to extract $\text{Br}^{(-)}$, $\text{I}^{(-)}$, $\text{Cl}^{(-)}$ from aq. soln. by gc

References: