



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

Synonym(s): *N,N,N*-Trimethyloctadecanaminium, 9Cl

CAS Registry Number: 15461-40-2

$\text{H}_3\text{C}(\text{CH}_2)_{17}\text{N}^{(+)}\text{Me}_3$

Molecular Formula:  $\text{C}_{21}\text{H}_{46}\text{N}^{(+)}$

Molecular Weight: 312.601

Accurate Mass: 312.363024

Percentage Composition: C 80.69%; H 14.83%; N 4.48%

>>Derivative: Chloride

Synonym(s): Trimethyloctadecylammonium chloride. Boraquat P30

CAS Registry Number: 112-03-8

Molecular Formula:  $\text{C}_{21}\text{H}_{46}\text{ClN}$

Molecular Weight: 348.054

Accurate Mass: 347.331876

Percentage Composition: C 72.47%; H 13.32%; Cl 10.19%; N 4.02%

Use/Importance: Surfactant. Used. in cosmetics

Physical Description: Cryst.

Melting Point: Mp 220 dec.°

Fluka: 74766

>>Derivative: Bromide

CAS Registry Number: 1120-02-1

Molecular Formula:  $\text{C}_{21}\text{H}_{46}\text{BrN}$

Molecular Weight: 392.505

Accurate Mass: 391.30136

Percentage Composition: C 64.26%; H 11.81%; Br 20.36%; N 3.57%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 250 dec.°

Aldrich: 35924-6

Fluka: 74765

>>Derivative: Iodide

CAS Registry Number: 4292-25-5

Molecular Formula:  $\text{C}_{21}\text{H}_{46}\text{IN}$

Molecular Weight: 439.506

Accurate Mass: 439.267497

Percentage Composition: C 57.39%; H 10.55%; I 28.87%; N 3.19%

Physical Description: Cryst.

Melting Point: Mp 227-230°

#### References:

Baltzly, R. *et al.*, *J.A.C.S.*, 1942, **64**, 2514, (*iodide*)

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

Celia, J.A. *et al.*, *J.A.C.S.*, 1952, **74**, 2061, (*chloride*)

Sprintschnik, G. *et al.*, *J.A.C.S.*, 1977, **99**, 4947, (*bromide*)

Isa, K. *et al.*, *Org. Mass Spectrom.*, 1983, **18**, 229, (*ms*)