



>>Entry Name: Dimethyldioctadecylammonium(1+)

Synonym(s): *N,N*-Dimethyl-*N*-octadecyl-1-octadecanaminium, 9Cl

CAS Registry Number: 14357-21-2

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

Molecular Formula: $\text{C}_{38}\text{H}_{80}\text{N}^{(+)}$

Molecular Weight: 551.057

Accurate Mass: 550.629074

Percentage Composition: C 82.83%; H 14.63%; N 2.54%

>>Derivative: Chloride

CAS Registry Number: 107-64-2

Molecular Formula: $\text{C}_{38}\text{H}_{80}\text{ClN}$

Molecular Weight: 586.509

Accurate Mass: 585.597926

Percentage Composition: C 77.82%; H 13.75%; Cl 6.04%; N 2.39%

Use/Importance: Surfactant. Used in hair preps. and fabric softeners

Physical Description: Cryst.

Melting Point: Mp 149-151°

>>Derivative: Bromide

CAS Registry Number: 3700-67-2

Molecular Formula: $\text{C}_{38}\text{H}_{80}\text{BrN}$

Molecular Weight: 630.961

Accurate Mass: 629.56741

Percentage Composition: C 72.34%; H 12.78%; Br 12.66%; N 2.22%

Use/Importance: Immunological adjuvant

Physical Description: Cryst. (MeCN)

Melting Point: Mp 161-163°

Aldrich: 38878-5

Sigma: D2779

References:

Swain, C.G. *et al.*, *J.A.C.S.*, 1955, **77**, 1122-1128, (*synth*)

Koenig, H. *et al.*, *Fresenius' Z. Anal. Chem.*, 1970, **251**, 225, (*nmr*)

Okuyama, L. *et al.*, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 1485-1490, (*bromide, cryst struct*)

Hilgers, L.A.T. *et al.*, *Res. Immunol.*, 1992, **143**, 494, (*rev, bromide, use*)