



>>Entry Name: Benzylododecyldimethylammonium(1+)

Synonym(s): *N*-Dodecyl-*N,N*-dimethylbenzenemethanaminium, 9Cl. Benzododecinium. Ajatin. Sterinol

CAS Registry Number: 10328-35-5

$\text{H}_3\text{C}(\text{CH}_2)_{11}\text{N}^{(+)}\text{Me}_2\text{CH}_2\text{Ph}$

Molecular Formula: $\text{C}_{21}\text{H}_{38}\text{N}^{(+)}$

Molecular Weight: 304.538

Accurate Mass: 304.300424

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

>>Derivative: Bromide

Synonym(s): Cequartyl 50

CAS Registry Number: 7281-04-1

Molecular Formula: $\text{C}_{21}\text{H}_{38}\text{BrN}$

Molecular Weight: 384.442

Accurate Mass: 383.23876

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

Use/Importance: Used as 10% aq. soln. for photometric detn. of Be (λ_{max} 610 nm, ϵ 105000); extraction of V(*V*) (C_6H_6 /octanol, pH 3.8), $[\text{Fe}(\text{CN})_6]^{4(-)}$; extraction of Prussian blue. Phase-transfer catalyst

Biological Use/Importance: Disinfectant and antiseptic

Physical Description: Cryst.

Melting Point: Mp 47°

Solubility: Sol. H_2O , acids; spar. sol. EtOH; insol. CCl_4

Hazard & Toxicity: LD₅₀ (rat, orl) 250 mg/kg

Aldrich: 28088-7

Fluka: 13375

Sigma: B5776

>>Derivative: Chloride

Synonym(s): Benzododecinium chloride, INN. Catiolite BC50. Cequartyl A. Dyk 1125. Noranium DA50. Orthosan HM. Tetranil BC80. Vantoc CL. Zephirol

CAS Registry Number: 139-07-1

Molecular Formula: $\text{C}_{21}\text{H}_{38}\text{ClN}$

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 31-32°

Hazard & Toxicity: Eye and skin irritant

Fluka: 13380

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 673A, (nmr)

Cella, J.A. *et al.*, *J.A.C.S.*, 1952, **74**, 2061-2062, (synth, activity)

Stepanenko, B.N. *et al.*, *CA*, 1968, **69**, 106057, (synth)

Namba, Y. *et al.*, *CA*, 1971, **74**, 125014, (synth)

Bartecki, A. *et al.*, *Nukleonika*, 1973, **18**, 71-81; *CA*, **79**, 35617q, (detn, V)

Galik, A. *et al.*, *Talanta*, 1974, **21**, 307-310, (use)

Palecek, J. *et al.*, *Synthesis*, 1976, 550-551, (use)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1979, **7**, 16, (use)

Kwapulińska, G. *et al.*, *Mikrochim. Acta*, 1984, **No. 1**, 333-338, (detn, Be)

He, H., *CA*, 1986, **104**, 206795, (synth)

Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, 1987, 6402

Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, 1993, 786

Rodier, N. *et al.*, *Acta Cryst. C*, 1995, **51**, 954-956, (cryst struct)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BEM000; BEO000