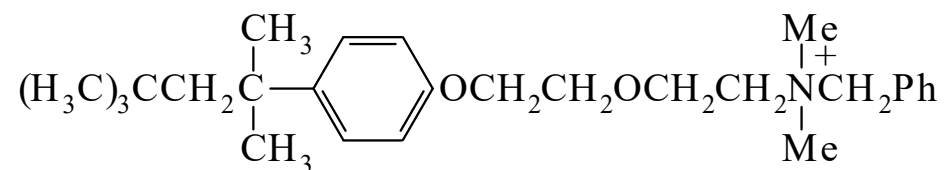




>>Entry Name: Benzethonium(1+)

Synonym(s): *N,N*-Dimethyl-*N*-[2-[2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethoxy]ethyl]benzenemethanaminium(1+), 9Cl. Benzyldimethyl[2-[2-(*p*-1,1,3,3-tetramethylbutylphenoxy)ethoxy]ethyl]ammonium. Hyamine 1622. Diisobutylphenoxyethoxyethyltrimethylbenzylammonium(1+). Many other names



CAS Registry Number: 10172-60-8

Extra CAS Registry Numbers(s): 5929-09-9

Molecular Formula: C₂₇H₄₂NO₂⁽⁺⁾

Molecular Weight: 412.634

Accurate Mass: 412.321554

Percentage Composition: C 78.59%; H 10.26%; N 3.39%; O 7.75%

>>Derivative: Chloride

Synonym(s): Benzethonium chloride, BAN, INN, USAN. Phemerol chloride

CAS Registry Number: 121-54-0

Molecular Formula: C₂₇H₄₂ClNO₂

Molecular Weight: 448.087

Accurate Mass: 447.290406

Percentage Composition: C 72.37%; H 9.45%; Cl 7.91%; N 3.13%; O 7.14%

Use/Importance: Used as aq. soln. for extraction separation of Th, Zr, Mo, Fe, Zn, Cd; extraction-photometric detn. of Co (as SCN complex, C₆H₆). Topical antiinfective agent. Vaginal spermicide. Antiseptic detergent. Preservative

Physical Description: Plates + 1H₂O (CHCl₃/Et₂O)

Melting Point: Mp 164-166°. Mp 184-186°

Solubility: V. sol. H₂O; sol. Me₂CO, EtOH, CHCl₃

Hazard & Toxicity: Severe eye irritant. LD₅₀ (rat, orl) 368 mg/kg

Aldrich: B470-8

Fluka: 53751

Sigma: B8879

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1322C, (ir)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 674C, (nmr)

Rawlins, A.L. *et al.*, *J. Am. Pharm. Assoc.*, 1943, **32**, 11

Finnegan, J.K. *et al.*, *J. Pharmacol. Exp. Ther.*, 1953, **109**, 422, (pharmacol)

Wilson, A.M. *et al.*, *Anal. Chem.*, 1962, **34**, 203, (rev)

Gundersen, N. *et al.*, *Anal. Chim. Acta*, 1968, **42**, 330, (use)

El-Yamani, I.S. *et al.*, *Talanta*, 1978, **25**, 714; 1984, **31**, 627, (detn, Zr, Th)

Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, 1987, 7603, (synonyms)

Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 30-31

Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1118

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BEN000