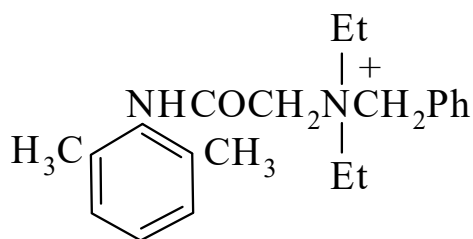




>>Entry Name: Denatonium(1+)

Synonym(s): *N*-[2-[(2,6-Dimethylphenyl)amino]-2-oxoethyl]-*N,N*-diethylbenzenemethanaminium, 9Cl. Benzyl-diethyl-[(2,6-xylyl-carbamoyl)methyl]ammonium, 8Cl



Molecular Formula: $C_{21}H_{29}N_2O^{+}$

Molecular Weight: 325.473

Accurate Mass: 325.227988

Percentage Composition: C 77.50%; H 8.98%; N 8.61%; O 4.92%

>>Derivative: Benzoate

Synonym(s): Denatonium benzoate, BAN, INN, USAN. Lidocaine benzylbenzoate. Bitrex. Denaton. Indigestin. NSC 157658. THS 839. Win 16568. BitterGuard

CAS Registry Number: 3734-33-6

Molecular Formula: $C_{28}H_{34}N_2O_3$

Molecular Weight: 446.588

Accurate Mass: 446.256943

Percentage Composition: C 75.31%; H 7.67%; N 6.27%; O 10.75%

Use/Importance: Denaturant for alcohol used in toiletries; deterrent to ingestion of toxic substances

Physical Description: Bitter-tasting cryst. (EtOAc/2-propanol)

Melting Point: Mp 166-170°

Solubility: Sol. H_2O , insol. Et_2O

Hazard & Toxicity: LD₅₀ (rat, orl) 584 mg/kg

Aldrich: 34853-8

Fluka: 30914

Rare Chemicals Library: S51043-2

Sigma: D5765

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 1367C, (*nmr*)

U.S. Pat., 1962, *T. + H. Smith*, 3 080 327; *CA*, **59**, 7429, (*synth*)

Glover, M.J. *et al.*, *Analyst (London)*, 1972, **97**, 891, (*use*)

Fr. Pat., 1982, *Glaxo*, 2 504 922; *CA*, **99**, 38064, (*synth, cryst, struct*)

Berning, C.K. *et al.*, *Fundam. Appl. Toxicol.*, 1982, **2**, 44, (*use*)

Hansen, S.R. *et al.*, *Vet. Hum. Toxicol.*, 1993, **35**, 234, (*tox*)

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