



>>Entry Name: **Dodecyldimethyl(2-phenoxyethyl)ammonium(1+)**

Synonym(s): *N,N*-Dimethyl-*N*-(2-phenoxyethyl)-1-dodecanaminium, 9Cl. Phenododecinium. Domiphen. Fungitex

CAS Registry Number: 13900-14-6

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

Molecular Formula: $\text{C}_{22}\text{H}_{40}\text{NO}^{(+)}$

Molecular Weight: 334.564

Accurate Mass: 334.310989

Percentage Composition: C 78.98%; H 12.05%; N 4.19%; O 4.78%

>>Derivative: Bromide

Synonym(s): **Domiphen bromide**, BAN, INN, USAN. Bradosol. Domibrom. NSC 39415. Many other names

CAS Registry Number: 538-71-6

Type of Compound Code(s): XA2200 XA1150 XA1550

Molecular Formula: $\text{C}_{22}\text{H}_{40}\text{BrNO}$

Molecular Weight: 414.468

Accurate Mass: 413.249325

Percentage Composition: C 63.75%; H 9.73%; Br 19.28%; N 3.38%; O 3.86%

Use/Importance: Used to treat minor infections of mouth and throat. Bactericide used in detergents and antiseptics

Melting Point: Mp 112-113°

Hazard & Toxicity: LD₅₀ (rat, ipr) 40 mg/kg

Aldrich: 24748-0

References:

U.S. Pat., 1952, 2 581 336; *CA*, **46**, 3713, (*synth, pharmacol*)

Gautier, J.A. *et al.*, *Bull. Soc. Chim. Fr.*, 1957, 1014, (*synth*)

U.S. Pat., 1975, 4 098 877; *CA*, **89**, 204264

Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, 1987, 6778, (*synonyms*)

Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, 1993, 794

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DXX000