



>>Entry Name: **Diphenhydramine**, BAN, INN

Synonym(s): 2-(Diphenylmethoxy)-*N,N*-dimethylethanamine, 9Cl. 2-(Diphenylmethoxy)-*N,N*-dimethylethylamine, 8Cl. Benzhydryl 2-dimethylaminoethyl ether. 2-Dimethylaminoethyl α -phenylbenzyl ether. Benzhydramine. Many other names

CAS Registry Number: 58-73-1

Related CAS Registry Numbers(s): 13168-00-8 15350-99-9

Type of Compound Code(s): XA4510

Ph2CHOCH2CH2NMe2

Molecular Formula: C₁₇H₂₁NO

Molecular Weight: 255.359

Accurate Mass: 255.162314

Percentage Composition: C 79.96%; H 8.29%; N 5.49%; O 6.27%

Use/Importance: Histamine H₁-receptor antagonist

Physical Description: Oil

Boiling Point: Bp₃ 163-167°. Bp₂ 150-165°

Calculated Log P Data: Log P 3.36 (calc)

Other Data: Component of Mandrax

Hazard & Toxicity: LD₅₀ (rat, orl) 390 mg/kg. Exp. reprod. effects

>>Derivative: Hydrochloride

Synonym(s): **Diphenhydramine hydrochloride**, USAN. Histex. Bendylate. Eldadryl. Benadryl. Dimedrol

CAS Registry Number: 147-24-0

Type of Compound Code(s): PA4750 PS8300

Use/Importance: Component of numerous proprietary preparations. Used as 2% aq. soln. in photometric detn. of Ti (ϵ 82000)

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 161-162°. Mp 166-170°

Solubility: Sol. H₂O

Hazard & Toxicity: Symptoms from overdosage (e.g. delirium, hallucinations) have been seen following topical use in children. LD₅₀ (rat, orl) 500 mg/kg. Exp. reprod. and teratogenic effects

Aldrich: 28566-8

Rare Chemicals Library: S40347-4

Sigma: D7774

>>Derivative: Citrate

Synonym(s): **Diphenhydramine citrate**, USAN

CAS Registry Number: 88637-37-0

>>Derivative: 8-Chlorotheophylline salt (1:1)

Synonym(s): Diphenhydramine teoclate. **Dimenhydrinate**, BAN, INN. Dramamine. Eldodram. Gravol. Many other names

CAS Registry Number: 523-87-5

Type of Compound Code(s): XA1500

Molecular Formula: C₂₄H₂₈ClN₅O₃

Molecular Weight: 469.97

Accurate Mass: 469.188067

Percentage Composition: C 61.34%; H 6.00%; Cl 7.54%; N 14.90%; O 10.21%

Use/Importance: Antinauseant

Melting Point: Mp 102-107°

Solubility: Sl. sol. H₂O

Hazard & Toxicity: LD₅₀ (rat, orl) 1320 mg/kg

Sigma: D2396