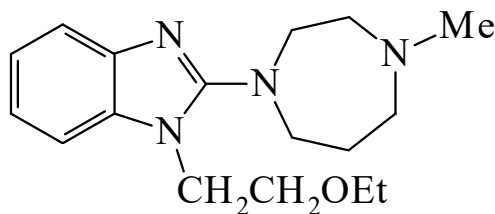




>>Entry Name: Emedastine, INN

Synonym(s): 1-(2-Ethoxyethyl)-2-(hexahydro-4-methyl-1*H*-1,4-diazepin-1-yl)-1*H*-benzimidazole. 1-(2-Ethoxyethyl)-2-(4-methyl-1-homopiperaziny)benzimidazole. Daren. Remicut



CAS Registry Number: 87233-61-2

Type of Compound Code(s): XA0950 XA4510

Molecular Formula: C₁₇H₂₆N₄O

Molecular Weight: 302.419

Accurate Mass: 302.210661

Percentage Composition: C 67.52%; H 8.67%; N 18.53%; O 5.29%

Use/Importance: Inhibits histamine release. Antiallergic, antiasthmatic agent showing low toxicity in exp. animals. Used in the treatment of allergic conjunctivitis

Physical Description: Oil

Development Status: Launched 1993 (Japan)

Calculated Log P Data: Log P 3.06 (calc)

>>Derivative: Fumarate (1:2)

Synonym(s): Emedastine difumarate, USAN. AL 3432A. KB 2413. LY 188695

CAS Registry Number: 87233-62-3

Molecular Formula: C₂₅H₃₄N₄O₉

Molecular Weight: 534.565

Accurate Mass: 534.232581

Percentage Composition: C 56.17%; H 6.41%; N 10.48%; O 26.94%

Physical Description: Needles (EtOAc/EtOH)

Melting Point: Mp 141-143°

Hazard & Toxicity: LD₅₀ (rat, orl) 1854 mg/kg. LD₅₀ (rat, scu) 643 mg/kg. LD₅₀ (rat, ivn) 72 mg/kg

>>Derivative: *N*-Oxide

Physical Description: Cryst. (DMF/EtOH) (as dipicrate)

Melting Point: Mp 87-193° (dipicrate)

References:

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Hamada, T. *et al.*, *Chem. Pharm. Bull.*, 1986, **34**, 1168, (*glc*)

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Iemura, R. *et al.*, *Chem. Pharm. Bull.*, 1989, **37**, 962; 967, (*metab*)

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