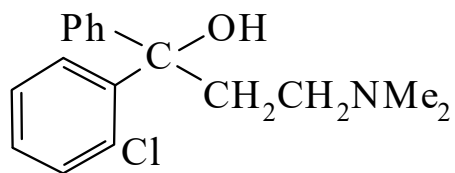




>>**Entry Name: Clofedanol**, INN

Synonym(s): 2-Chloro- α -[2-(dimethylamino)ethyl]- α -phenylbenzenemethanol, 9CI. 1-*o*-Chlorophenyl-3-dimethylamino-1-phenylpropanol. **Chlophedianol**, BAN. Bayer 186. Calmotusin. Many other names



CAS Registry Number: 791-35-5

Molecular Formula: C₁₇H₂₀ClNO

Molecular Weight: 289.804

Accurate Mass: 289.123341

Percentage Composition: C 70.46%; H 6.96%; Cl 12.23%; N 4.83%; O 5.52%

Use/Importance: Antitussive

Calculated Log P Data: Log P 2.76 (calc)

Hazard & Toxicity: LD₅₀ (mus, orl) 300 mg/kg

>>**Variant: (+)-form**

Molecular Formula: C₁₇H₂₀ClNO

Molecular Weight: 289.804

Accurate Mass: 289.123341

Percentage Composition: C 70.46%; H 6.96%; Cl 12.23%; N 4.83%; O 5.52%

Melting Point: Mp 115-116.5°

Optical Rotation: [α]_D +22.3 (CHCl₃)

Other Data: Abs. config. apparently not detd. (1994)

>>**Derivative:** Hydrochloride

Melting Point: Mp 172-175°

Optical Rotation: [α]_D +9

>>**Variant: (±)-form**

Molecular Formula: C₁₇H₂₀ClNO

Molecular Weight: 289.804

Accurate Mass: 289.123341

Percentage Composition: C 70.46%; H 6.96%; Cl 12.23%; N 4.83%; O 5.52%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 120-121°

>>**Derivative:** Hydrochloride

Synonym(s): **Chlophedianol hydrochloride**, BAN, USAN. Clofedanol hydrochloride, JAN. Detigon

CAS Registry Number: 511-13-7

Melting Point: Mp 190-191°

Sigma: C2165

References:

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Unterhalt, B. *et al.*, *Pharm. Ztg.*, 1974, **119**, 769, (*ir, pmr, anal*)
Eckhardt, G. *et al.*, *J. Clin. Chem. Clin. Biochem.*, 1977, **15**, 687, (*metab*)
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, 1987, 4399, (*synonyms*)
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