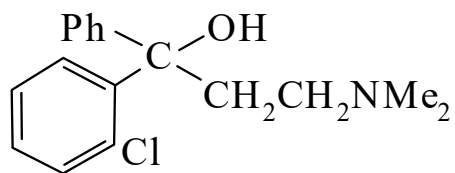




>>**Entry Name:** Clofedanol, INN

Synonym(s): 2-Chloro- α -[2-(dimethylamino)ethyl]- α -phenylbenzenemethanol, 9Cl. 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:

- Goeswald, R., *Arzneim.-Forsch.*, 1958, **8**, 550, (*pharmacol*)
Fles, D. *et al.*, *Croat. Chem. Acta*, 1960, **32**, 209, (*synth, resoln*)
Chen, J.Y.P. *et al.*, *J. Pharmacol. Exp. Ther.*, 1960, **128**, 384, (*pharmacol*)
Henecka, H. *et al.*, *CA*, 1964, **60**, 4121h, (*synth, resoln*)
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*)
Martindale, *The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, 1993, 745
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, CMW700