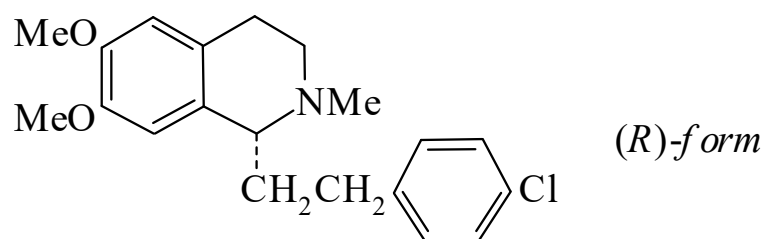




>>>**Entry Name:** Metofoline, BAN, INN

Synonym(s): 1-[2-(4-Chlorophenyl)ethyl]-1,2,3,4-tetrahydro-6,7-dimethoxy-2-methylisoquinoline, 9Cl. 1-(*p*-Chlorophenethyl)-1,2,3,4-tetrahydro-6,7-dimethoxy-2-methylisoquinoline, 8Cl. **Methopholine**, USAN. Versidyne. ARC I-K-1. NIH 7672. Ro 4-1778



CAS Registry Number: 2154-02-1

Molecular Formula: C₂₀H₂₄ClNO₂

Molecular Weight: 345.868

Accurate Mass: 345.149556

Percentage Composition: C 69.45%; H 6.99%; Cl 10.25%; N 4.05%; O 9.25%

Use/Importance: Analgesic

Development Status: No longer marketed

Calculated Log P Data: Log P 4.97 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 400 mg/kg. LD₅₀ (rat, ipr) 100 mg/kg

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

Molecular Formula: C₂₀H₂₄ClNO₂

Molecular Weight: 345.868

Accurate Mass: 345.149556

Percentage Composition: C 69.45%; H 6.99%; Cl 10.25%; N 4.05%; O 9.25%

Melting Point: Mp 79-80°

Boiling Point: Bp_{0.15} 194°

Optical Rotation: [α]_D²⁵ -16 (c, 1.0 in MeOH)

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

Molecular Formula: C₂₀H₂₄ClNO₂

Molecular Weight: 345.868

Accurate Mass: 345.149556

Percentage Composition: C 69.45%; H 6.99%; Cl 10.25%; N 4.05%; O 9.25%

Boiling Point: Bp_{0.06} 196-198°

Optical Rotation: [α]_D²⁵ +17.9 (c, 1.0 in MeOH)

>>>**Variant:** (±)-form

Molecular Formula: C₂₀H₂₄ClNO₂

Molecular Weight: 345.868

Accurate Mass: 345.149556

Percentage Composition: C 69.45%; H 6.99%; Cl 10.25%; N 4.05%; O 9.25%

Melting Point: Mp 109-110°

>>>**Derivative:** Hydrochloride

Melting Point: Mp 105-106°

References:

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Besendorf, H. *et al.*, *Experientia*, 1962, **18**, 446, (*pharmacol*)

Jirkovsky, I. *et al.*, *Coll. Czech. Chem. Comm.*, 1967, **32**, 1197, (*synth, deriv*)

Sciorelli, G. *et al.*, *Experientia*, 1967, **23**, 934, (*metab*)

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