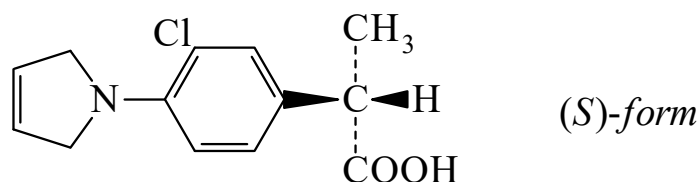




>>Entry Name: Pirprofen, BAN, INN, USAN

Synonym(s): 3-Chloro-4-(2,5-dihydro-1H-pyrrol-1-yl)- α -methylbenzeneacetic acid, 9Cl. 2-[3-Chloro-4-(3-pyrrolin-1-yl)phenyl]propionic acid. Rangasil. Rengacil. SU 21524. Rengasil



CAS Registry Number: 31793-07-4

Related CAS Registry Numbers(s): 50537-15-0

Molecular Formula: C₁₃H₁₄ClNO₂

Molecular Weight: 251.712

Accurate Mass: 251.071306

Percentage Composition: C 62.03%; H 5.61%; Cl 14.08%; N 5.56%; O 12.71%

Use/Importance: Analgesic. Antiinflammatory agent

Development Status: No longer marketed

Calculated Log P Data: Log P 2.55 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 351 mg/kg. LD₅₀ (rat, ivn) 167 mg/kg. Hepatotoxicity reported

>>Variant: (S)-form

CAS Registry Number: 32655-63-3

Molecular Formula: C₁₃H₁₄ClNO₂

Molecular Weight: 251.712

Accurate Mass: 251.071306

Percentage Composition: C 62.03%; H 5.61%; Cl 14.08%; N 5.56%; O 12.71%

Boiling Point: Bp 255° approx.

Optical Rotation: $[\alpha]_D^{25} +38.08$ (EtOH)

>>Derivative: Na salt

Melting Point: Mp 214-216°

Optical Rotation: $[\alpha]_D^{25} -17.38$

>>Variant: (±)-form

Molecular Formula: C₁₃H₁₄ClNO₂

Molecular Weight: 251.712

Accurate Mass: 251.071306

Percentage Composition: C 62.03%; H 5.61%; Cl 14.08%; N 5.56%; O 12.71%

Physical Description: Cryst. (C₆H₆/hexane)

Melting Point: Mp 98-100°

>>Derivative: Et ester

Molecular Formula: C₁₅H₁₈ClNO₂

Molecular Weight: 279.765

Accurate Mass: 279.102606

Percentage Composition: C 64.40%; H 6.48%; Cl 12.67%; N 5.01%; O 11.44%

Boiling Point: Bp_{0.25} 128-133°

References:

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Liang, W.T.C. *et al.*, *J. Chromatogr.*, 1992, **577**, 317, (*hplc, enantiomers*)

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