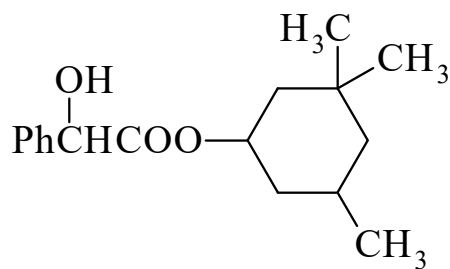




>>Entry Name: **Cyclandelate**, BAN, INN, JAN

Synonym(s): 3,3,5-Trimethylcyclohexyl α -hydroxybenzeneacetate, 9CI. 3,3,5-Trimethylcyclohexyl mandelate, 8CI. Capilan. Cyclobral. Cyclospasmol. BS 572. Many other names



CAS Registry Number: 456-59-7

Molecular Formula: C₁₇H₂₄O₃

Molecular Weight: 276.375

Accurate Mass: 276.172545

Percentage Composition: C 73.88%; H 8.75%; O 17.37%

Biological Use/Importance: Antispasmodic, vasodilator

Melting Point: Mp 50-53°

Boiling Point: Bp₁₄ 192-194°

Solubility: Insol. H₂O

Calculated Log P Data: Log P 4.64 (calc)

Other Data: Stereochem. not defined

Hazard & Toxicity: LD₅₀ (rat, orl) 5000 mg/kg

Sigma: C9260

>>Derivative: 3-Pyridinecarboxylate

see Micinicate, [BNZ45-H](#)

References:

- Brock, N. *et al.*, *Arzneim.-Forsch.*, 1952, **2**, 165, (*synth*)
van den Akker, S. *et al.*, *Arzneim.-Forsch.*, 1957, **7**, 15, (*pharmacol*)
Ernsting, M.J.E. *et al.*, *Arzneim.-Forsch.*, 1962, **12**, 632; 691; 853, (*metab*)
Ernsting, M.J.E. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1962, **81**, 751, (*synth*)
Doorendos, H.J. *et al.*, *Pharm. Weekbl.*, 1965, **100**, 633, (*pharmacol*)
van der Vlies, C. *et al.*, *Pharm. Weekbl.*, 1966, **101**, 93, (*nmr*)
Kracmar, J. *et al.*, *Pharmazie*, 1976, **31**, 363, (*uv*)
Amano, T. *et al.*, *Chem. Pharm. Bull.*, 1981, **29**, 1106, (*cmr, ir, glc*)
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, 1987, 4531
Shearer, C.M., *Anal. Profiles Drug Subst.*, 1992, **21**, 149, (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1309
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DNU100