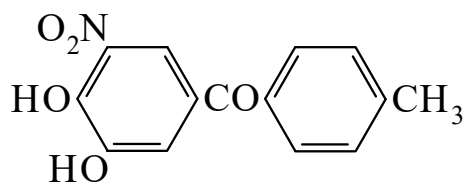




>>Entry Name: 3,4-Dihydroxy-4'-methyl-5-nitrobenzophenone

Synonym(s): (3,4-Dihydroxy-5-nitrophenyl)(4-methylphenyl)methanone, 9CI. **Tolcapone**, BAN, INN, USAN. Tasmar. Ro 40-7592



CAS Registry Number: 134308-13-7

Molecular Formula: C₁₄H₁₁NO₅

Molecular Weight: 273.245

Accurate Mass: 273.063724

Percentage Composition: C 61.54%; H 4.06%; N 5.13%; O 29.28%

Use/Importance: Catechol-*O*-methyltransferase inhibitor. Used in combination therapy with 2-Amino-3-(3,4-dihydroxyphenyl)propanoic acid [HHZ68-O](#) in treatment of Parkinson's disease

Physical Description: Yellow cryst.

Development Status: Approved by FDA (1998)

Melting Point: Mp 144-145°

Calculated Log P Data: Log P 3.21 (calc)

Hazard & Toxicity: LD₅₀ (mus, orl) 1600 mg/kg

References:

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