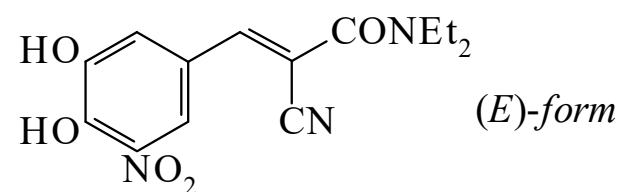




>>Entry Name: Entacapone, BAN, INN, USAN

Synonym(s): 2-Cyano-3-(3,4-dihydroxy-5-nitrophenyl)-N,N-diethyl-2-propenamide, 9Cl. Comtan. Comtess. OR-611



Related CAS Registry Numbers(s): 116314-67-1 145195-63-7

Type of Compound Code(s): XA2050

Molecular Formula: C₁₄H₁₅N₃O₅

Molecular Weight: 305.29

Accurate Mass: 305.101172

Percentage Composition: C 55.08%; H 4.95%; N 13.76%; O 26.20%

Use/Importance: Catechol-O-methyltransferase inhibitor. Antiparkinsonian agent

Development Status: Launched in Finland, Germany and Sweden (1998)

>>Variant: (E)-form

CAS Registry Number: 130929-57-6

Molecular Formula: C₁₄H₁₅N₃O₅

Molecular Weight: 305.29

Accurate Mass: 305.101172

Percentage Composition: C 55.08%; H 4.95%; N 13.76%; O 26.20%

Melting Point: Mp 162-163°

>>Variant: (Z)-form

Molecular Formula: C₁₄H₁₅N₃O₅

Molecular Weight: 305.29

Accurate Mass: 305.101172

Percentage Composition: C 55.08%; H 4.95%; N 13.76%; O 26.20%

Melting Point: Mp 148-151°

Other Data: Readily converts to more stable (E)-form in the presence of acids or heat

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