Entacapone
Item No. 14153

CAS Registry No.: 130929-57-6
Formal Name: 2-cyano-3-(3,4-dihydroxy-5-nitrophenyl)-N,N-dieethyl-2E-propenamide
Synonyms: Comtan, OR 611
MF: C_{14}H_{15}N_{3}O_{5}
FW: 305.3
Purity: ≥98%
Stability: ≥2 years at -20°C
Supplied as: A crystalline solid
UV/Vis: \( \lambda_{\text{max}} = 224, 309 \text{ nm} \)

Laboratory Procedures

For long term storage, we suggest that entacapone be stored as supplied at -20°C. It should be stable for at least two years.

Entacapone is supplied as a crystalline solid. A stock solution may be made by dissolving the entacapone in the solvent of choice. Entacapone is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of entacapone in ethanol is approximately 5 mg/ml and approximately 30 mg/ml in DMSO and DMF.

Entacapone is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, entacapone should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Entacapone has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Catechol O-methyltransferase (COMT) is a key enzyme involved in the degradation of catecholamines including dopamine, epinephrine, and norepinephrine. COMT metabolizes L-3,4-dihydroxyphenylalanine (L-DOPA) to 3-O-methyldopa (3-OMD), and then further to vanillactic acid, which is excreted in urine. Entacapone is a peripherally acting, selective and reversible COMT inhibitor with IC\(_{50}\) values of 150-300 nM in rat liver (K\(_{i}\) = 145 nM) and 3-O-methyldopa (3-OMD), and then further to vanillactic acid, which is excreted in urine. Entacapone is a peripherally acting, selective and reversible COMT inhibitor with IC\(_{50}\) values of 150-300 nM in rat liver (K\(_{i}\) = 145 nM) and 10-20 nM in rat brain tissues. It was designed as an adjuvant to L-DOPA/dopa decarboxylase inhibitor treatment for Parkinson's disease. Peripheral COMT inhibition with entacapone can decrease 3-OMD levels in the rat brain by 16-52% and prolong the bioavailability of L-DOPA in patients with Parkinson's disease.

References

Related Products
For a list of related products please visit: www.caymanchem.com/catalog/14153

WARNING: THIS PRODUCT IS FOR LABORATORY RESEARCH ONLY: NOT FOR ADMINISTRATION TO HUMANS. NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA
This material should be considered hazardous until information to the contrary becomes available. Do not ingest, swallow, or inhale. Do not get in eyes, on skin, or on clothing. Wash thoroughly after handling. This information contains some, but not all, of the information required for the safe and proper use of this material. Before use, the user must review the complete Safety Data Sheet, which has been sent to our email at your institution.

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