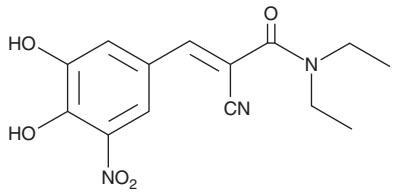
# PRODUCT INFORMATION

## Entacapone

*Item No. 14153*

**CAS Registry No.:** 130929-57-6
**Formal Name:** 2-cyano-3-(3,4-dihydroxy-5-nitrophenyl)-N,N-diethyl-2E-propenamide
**Synonym:** OR-611
**MF:** $C_{14}H_{15}N_3O_5$
**FW:** 305.3
**Purity:** ≥98%
**UV/Vis.:** $\lambda_{max}$: 224, 309 nm
**Supplied as:** A crystalline solid
**Storage:** -20°C
**Stability:** ≥4 years




*Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.*

### Laboratory Procedures

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.

### Description

Entacapone is a reversible catechol O-methyltransferase (COMT) inhibitor ($IC_{50}$s = 10, 10, 20, and 160 nM for rat duodenum, brain, erythrocyte, and liver COMT, respectively).[1] It is selective for COMT over monoamine oxidase A (MAO-A) and MAO-B and phenolsulphotransferase M (PST-M) and PST-P ($IC_{50}$s = >50 µM). Entacapone (10 mg/kg), in combination with L-DOPA (Item No. 13248) and carbidopa (Item No. 23783), reduces 3-O-methyldopa (3-OMD) levels in the rat striatum and hypothalamus to 52 and 27%, respectively, of the levels in control animals receiving only L-DOPA and carbidopa.[2] In a 6-OHDA rat model of Parkinson's disease, entacapone (10 mg/kg), in combination with L-DOPA and benserazide (Item No. 20298), increases contralateral turning behavior and striatal extracellular dopamine levels.[3] Entacapone also inhibits contraction of colon longitudinal muscle explants from a 6-OHDA rat model of Parkinson's disease ($EC_{50}$ = 200 µM).[4] Formulations containing entacapone have been used in the treatment of Parkinson's disease.

### References


1. Nissinen, E., Lindén, I.B., Schultz, E., *et al. Naunyn Schmiedebergs Arch. Pharmacol.* **346(3)**, 262-266 (1992).
2. Männistö, P.T., Tuomainen, P., and Tuominen, R.K. *Br. J. Pharmacol.* **105(3)**, 569-574 (1992).
3. Gerlach, M., van den Buuse, M., Blaha, C., *et al. Naunyn Schmiedebergs Arch. Pharmacol.* **370(5)**, 388-394 (2004).
4. Li, L.-S., Liu, C.-Z., Xu, J.-D., *et al. World J. Gastroenterol.* **21(12)**, 3509-3518 (2015).





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