Product Data Sheet

Product Name: Entacapone sodium salt
Cat. No.: GC18091

Chemical Properties

Cas. No.	1047659-02-8		
Chemical Name	sodium (E)-5-(2-cyano-3-(diethylamino)-3-oxoprop-1-en-1-yl)-2-hydroxy-3-nitrophenolate		
SMILES	CCN(C(/C(C#N)=C([H])/C1=CC(N(=O)=O)=C(O)C([O-])=C1)=O)CC.[Na+]		
Formula	$C_{14}H_{14}N_3NaO_5$	M.Wt	327.27
Solubility	Soluble in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	Entacapone sodium salt		

Background

Entacapone, a nitrocatechol compound, is a selective and reversible inhibitor of catechol-O-methyltransferase (COMT), a Mg2+-dependent enzyme involved in the metabolism of catecholamines and catechol compounds, with the half maximal inhibition concentration IC50 and inhibition constant Ki values of 20.1 nM and 10.7 nM respectively [1 & 2].

The nitro group at the position ortho to the hydroxyl group in the chemical structure of entacapone has been identified as a critical component for its potency and ability to inhibit COMT [2].

Entacapone is an FDA-approved COMT inhibitor for use as an adjunct to levodopa therapy in patients' with Parkinson's disease, where it increases both the peripheral and central availability of levodopa [2].

Reference

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References:
[1] Forsberg M, Lehtonen M, Heikkinen M, Savolainen J, Järvinen T, Männistö PT. Pharmacokinetics and pharmacodynamics of entacapone and tolcapone after acute and repeated administration: a comparative study in the rat. J Pharmacol Exp Ther. 2003 Feb;304(2):498-506.
[2] Najib J. Entacapone: a catechol-O-methyltransferase inhibitor for the adjunctive treatment of Parkinson's disease. Clin Ther. 2001 Jun;23(6):802-32; discussion 771.

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