
Product Data Sheet

Product Name: Brexpiprazole S-oxide

Cat. No.: GC60662

Chemical Properties

Cas. No. 1191900-51-2

SMILES O=C1NC2=C(C=CC(OCCCCN3CCN(C4=C(C=CS5=O)C5=CC=C4)CC3)=C2)C=C1

Formula $C_{25}H_{27}N_3O_3S$ M.Wt 449.57

Solubility DMSO : 25 mg/mL (55.61 mM; Need ultrasonic) Storage Store at -20°C

General tips For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C 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

Background

Brexpiprazole S-oxide (DM-3411) is a main metabolite of Brexpiprazole and is metabolized by cytochrome P450 3A4 (CYP3A4). Brexpiprazole is an atypical antipsychotic agent and a partial agonist of human 5-HT1A and dopamine receptor with K_{is} of 0.12 nM and 0.3 nM, respectively. Brexpiprazole is also a 5-HT2A receptor antagonist with a K_i of 0.47 nM [1][2] [3].

[1]. Chen B, et al. Effects of 26 Recombinant CYP3A4 Variants on Brexpiprazole Metabolism. Chem Res Toxicol. 2019 Oct 17. [2]. Ishima T, et al. Potentiation of neurite outgrowth by brexpiprazole, a novel serotonin-dopamine activity modulator: a role for serotonin 5-HT1A and 5-HT2A receptors. Eur Neuropsychopharmacol. 2015 Apr;25(4):505-11. [3]. Yoshimi N, et al. Improvement of dizocilpine-induced social recognition deficits in mice by brexpiprazole, a novel serotonin-dopamine activity modulator. Eur Neuropsychopharmacol. 2015 Mar;25(3):356-64.

Caution: Product has not been fully validated for medical applications. For research use only.

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