

Certificate of Analysis

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Product Name: rac BHFF

Catalog No.: 3313

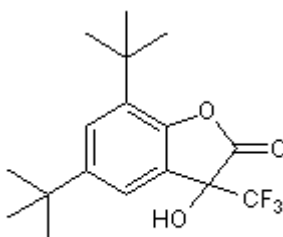
Batch No.: 1

CAS Number: 123557-91-5

IUPAC Name: 5,7-Bis(1,1-dimethylethyl)-3-hydroxy-3-(trifluoromethyl)-2(3H)-benzofuranone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₂₁F₃O₃
Batch Molecular Weight: 330.34
Physical Appearance: White solid
Solubility: DMSO to 100 mM
ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



C₁₇H₂₁F₃O₃
Mol. Wt.: 330.34

2. ANALYTICAL DATA

Melting Point: Between 88 - 89°C
HPLC: Shows >98.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical	61.81	6.41
Found	61.66	6.06

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Potent and selective GABA_B receptor positive allosteric modulator that increases the potency and efficacy of GABA (> 15-fold and > 149% respectively). Exhibits anxiolytic activity in vivo and is orally active.

Physical and Chemical Properties:

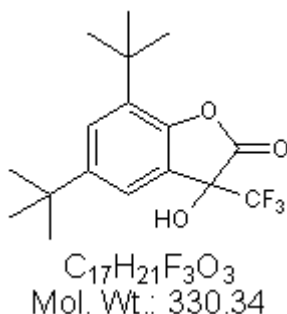
Batch Molecular Formula: C₁₇H₂₁F₃O₃

Batch Molecular Weight: 330.34

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Malherbe et al (2008) Characterization of (*R,S*)-5,7-di-*tert*-butyl-3-hydroxy-3-trifluoromethyl-3*H*-benzofuran-2-one as a positive allosteric modulator of GABA_B receptors. *Br.J.Pharmacol.* **154** 797. PMID: 18536733.

Koek et al (2013) Discriminative stimulus effects of the GABA_B receptor-positive modulator rac-BHFF: comparison with GABA_B receptor agonists and drugs of abuse. *J.Pharmacol.Exp.Ther.* **344** 553. PMID: 23275067.

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