

Certificate of Analysis

Product Name: DG 172 dihydrochloride

Catalog No.: 5566

Batch No.: 1

CAS Number: 1361504-77-9

IUPAC Name: (*αZ*)-2-Bromo-*α*-[[4-(4-methyl-1-piperazinyl)phenyl]methylene]benzeneacetonitrile dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₀BrN₃·2HCl

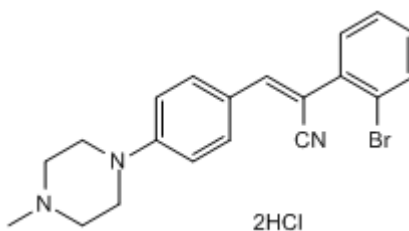
Batch Molecular Weight: 455.22

Physical Appearance: Pale yellow solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.52 (Dichloromethane:Methanol [95:5])

HPLC: Shows >99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.77	4.87	9.23
Found	52.84	4.91	9.22

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

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Description:

Potent PPAR β/δ inverse agonist (IC₅₀ = 26.9 nM). Inhibits Angptl4 gene expression in mouse myoblasts (IC₅₀ = 9.5 nM) in vitro. Also augments GM-CSF/IL-4-induced differentiation of mature dendritic cells from bone marrow cells in culture. Orally available.

Physical and Chemical Properties:

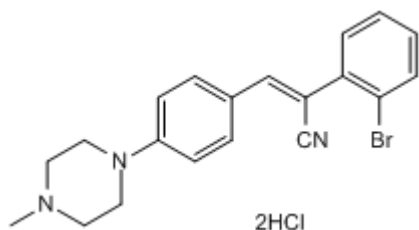
Batch Molecular Formula: C₂₀H₂₀BrN₃.2HCl

Batch Molecular Weight: 455.22

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM
DMSO 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:

Lieber *et al* (2012) (Z)-2-(2-bromophenyl)-3-[[4-(1-methyl-piperazine)amino]phenyl]acrylonitrile (DG172): an orally bioavailable PPAR β/δ -selective ligand with inverse agonistic properties. *J.Med.Chem.* **55** 2858. PMID: 22369181.

Lieber *et al* (2015) The inverse agonist DG172 triggers a PPAR β/δ -independent myeloid lineage shift and promotes GM-CSF/IL-4-induced dendritic cell differentiation. *Mol.Pharmacol.* **87** 162. PMID: 25398837.

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