

Certificate of Analysis

Print Date: Mar 9th 2022

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Product Name: PK 11195 Catalog No.: 0670 Batch No.: 11

CAS Number: 85532-75-8

IUPAC Name: 1-(2-Chlorophenyl)-N-methyl-N-(1-methylpropyl)-3-isoquinolinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

C₂₁H₂₁CIN₂O **Batch Molecular Formula:**

Batch Molecular Weight: 352.86 **Physical Appearance:** White solid

ethanol to 50 mM Solubility:

DMSO to 50 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

Melting Point: Between 136 - 138°C

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure **Mass Spectrum:** Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 71.48 6 7.94 Found 71.45 6.05 8.04



Product Information

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CAS Number: 85532-75-8

IUPAC Name: 1-(2-Chlorophenyl)-*N*-methyl-*N*-(1-methylpropyl)-3-isoquinolinecarboxamide

Description:

PK 11195 has high affinity for the peripheral benzodiazepine receptor (PBR, TSPO) without binding to other known neurotransmitter receptors. Also inhibits the human constitutive androstane receptor (hCAR).

Physical and Chemical Properties:

Batch Molecular Formula: C₂₁H₂₁CIN₂O Batch Molecular Weight: 352.86 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

ethanol to 50 mM DMSO to 50 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:

Li et al (2008) The peripheral benzodiazepine receptor ligand 1-(2-chlorophenyl-methylpropyl)-3-isoquinoline-carboxamide is a novel antagonist of human androstane receptor. Mol.Pharmacol. **74** 443. PMID: 18492798.

Conway et al (1998) Temporal changes in glial fibrillary acidic protein messenger RNA and [3H]PK11195 binding in relation to imidazoline-l2-receptor and α 2-adrenoceptor binding in the hippocampus following transient global forebrain isch Neuroscience 82 805. PMID: 9483537.

Le Fur *et al* (1983) Differentiation between two ligands for peripheral benzodiazpine binding sites [³H]-Ro 5-4864 and [³H]-PK11195, by thermodynamic studies. Life Sci. *33* 449. PMID: 6308375.