1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{21}\text{H}_{21}\text{ClN}_2\text{O} \)

Batch Molecular Weight: 352.86

Physical Appearance: White solid

Solubility: ethanol to 50 mM

DMSO to 50 mM

Storage: Store at RT

2. ANALYTICAL DATA

Melting Point: Between 136 - 138°C

HPLC: Shows 99.8% purity

\(^1\text{H NMR:} \) Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical: 71.48 \text{C} \ 6 \text{H} \ 7.94 \text{N}

Found: 71.45 \text{C} \ 6.05 \text{H} \ 8.04 \text{N}
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

**Description:**
Possesses 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:** C_{21}H_{23}ClN_{2}O
- **Batch Molecular Weight:** 352.86
- **Physical Appearance:** White solid
- **Minimum Purity:** ≥98%

**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:**