Product Name: (S)-(+) Ibuprofen  
Catalog No.: 2796  
Batch No.: 1

CAS Number: 51146-56-6  
IUPAC Name: (S)-α-Methyl-4-(2-methylpropyl)benzeneacetic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

- Batch Molecular Formula: \( \text{C}_{13}\text{H}_{18}\text{O}_{2} \)
- Batch Molecular Weight: 206.28
- Physical Appearance: White crystalline solid
- Solubility: DMSO to 100 mM, ethanol to 100 mM
- Storage: Store at RT

2. ANALYTICAL DATA

- Melting Point: Between 51 - 52°C
- HPLC: Shows >99.9% purity
- \(^1\)H NMR: Consistent with structure
- Mass Spectrum: Consistent with structure
- Optical Rotation: \([\alpha]_D = +61.7\) (Concentration = 0.6, Solvent = Methanol)
Product Name: (S)-(+-)Ibuprofen
CAS Number: 51146-56-6
IUPAC Name: (S)-α-Methyl-4-(2-methylpropyl)benzeneacetic acid

Description:
Non-steroidal anti-inflammatory drug (NSAID) that inhibits cyclooxygenase 1 and cyclooxygenase 2 (IC50 values are 12 and 80 μM respectively). Active isomer of ibuprofen.

Physical and Chemical Properties:
Batch Molecular Formula: C13H18O2
Batch Molecular Weight: 206.28
Physical Appearance: White crystalline solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

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: