1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** \( C_{32}H_{47}F_5O_3S \)
- **Batch Molecular Weight:** 606.77
- **Physical Appearance:** White solid
- **Solubility:**
  - Ethanol to 50 mM
  - DMSO to 100 mM
- **Storage:** Store at RT

2. ANALYTICAL DATA

- **HPLC:** Shows 99.7% purity
- **\(^1\)H NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:**
  - Carbon Hydrogen Nitrogen
  - Theoretical: 63.34 7.81
  - Found: 63.48 7.78
Product Name: ICI 182,780
Catalog No.: 1047  Batch No.: 21

CAS Number: 129453-61-8
IUPAC Name: 7α,17β-[9-[(4,4,5,5,5-Pentafluoropentyl)sulfinyl]nonyl]estra-1,3,5(10)-triene-3,17-diol

Description:
A high affinity estrogen receptor antagonist (IC_{50} = 0.29 nM), devoid of any partial agonism both in vitro and in vivo. Also high affinity agonist at the membrane estrogen receptor GPER.

Physical and Chemical Properties:
Batch Molecular Formula: C_{32}H_{40}F_{5}O_{3}S
Batch Molecular Weight: 606.77
Physical Appearance: White solid
Minimum Purity: >99%

Storage: Store at RT
Solubility & Usage Info:
ethanol to 50 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.

Licensing Information:
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References: