3050 Spruce Street, St. Louis, MO 63103 USA
Tel: (800) 521-8956 (314) 771-5765 Fax: (800) 325-5052 (314) 771-5757
email: techservice@sial.com sigma-aldrich.com

# **Product Information**

Secobarbital solution
1.0 mg/mL±5% in methanol
analytical standard, for drug analysis

Catalog Number **S4006**Lot Number SLBJ7469V
Storage Temperature 2–8 °C

CAS RN 76-73-3

Synonyms: Meballymal, Quinalbarbitone, 5-Allyl-5(1-methylbutyl)barbituric acid, 5-(1-Methylbutyl)-5-(2-propenyl)-2,4,6(1H,3H,5H)-pyrimidinetrione

**Product Description** 

Molecular Formula: C<sub>12</sub>H<sub>18</sub>N<sub>2</sub>O<sub>3</sub> Molecular Weight: 238.28

DEA Class: Exempt preparation of Class II

Concentration: 0.99 mg of secobarbital/mL of GC grade methanol, concentration verified by UV.

Expiration Date: April 2017

#### **Precautions and Disclaimer**

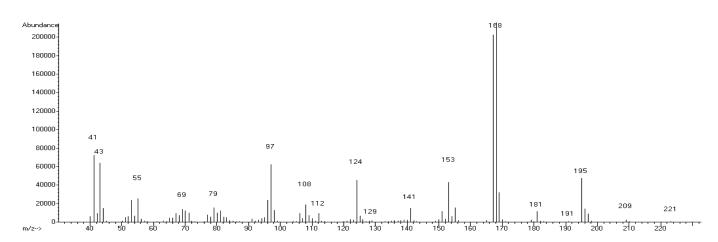
This product is for R&D use only, not for drug, household, or other uses. Please consult the Material Safety Data Sheet for information regarding hazards and safe handling practices.

## Storage/Stability

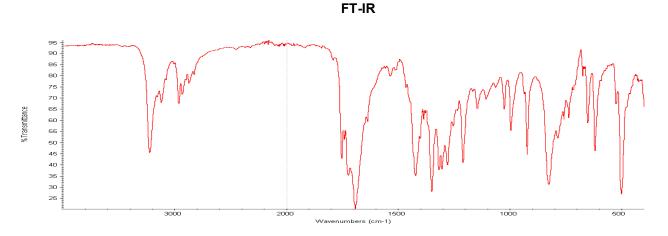
Store the product at 2–8  $^{\circ}$ C. If stored at 2–8  $^{\circ}$ C in an airtight container, protected from light, decomposition of the product is less than 1% in 48 months. After opening, concentration may change due to loss of solvent.

CMW,MAM 04/14-1

#### 70 eV Electron Ionization Mass Spectrum



Hewlett-Packard 6890 Series II Gas Chromatograph Hewlett-Packard 5973 Mass Selective Detector Hewlett-Packard G1701DA MS ChemStation (HP-DOS series)



Nicolet 380 FT-IR (Thermo Smart Orbit)

## **Ultraviolet Spectrum**

 Peak
 239.5 nm

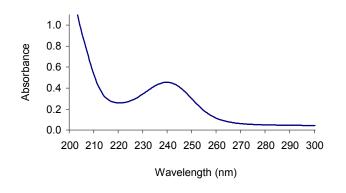
 Absorbance
 0.4553

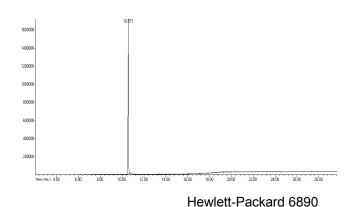
Solvent 50 mM Borax

**Dilution** 1:99 (v/v)

## **Capillary Gas Chromatography**

Column Supelco SPB-1 (Catalog Number 24162)
I.D. 0.20 mm Length 15 m Film Thickness 0.20 μm
Oven Temperature 50 °C (2 minutes), then
15 °C/minute to 300 °C, hold 11 minutes
Injector Temperature 250 °C, Split
Detector Hewlett-Packard 6890
Mass Selective Detector (70 eV, 40-500 m/z)





Beckman-Coulter DU 800

Deckman-Soulier Do 600