5-Fluoro MN-18

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

1. GENERAL INFORMATION

   **IUPAC Name:** 1-(5-fluoropentyl)-N-(naphthalen-1-yl)-1H-indazole-3-carboxamide

   **CAS#:** NA

   **Synonyms:** NA

   **Source:** DEA Reference Material Collection

   **Appearance:** Off-white powder

   **UV<sub>max</sub>(nm):** NA

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Melting Point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C&lt;sub&gt;23&lt;/sub&gt;H&lt;sub&gt;22&lt;/sub&gt;FN&lt;sub&gt;3&lt;/sub&gt;O</td>
<td>375</td>
<td>89.1</td>
</tr>
</tbody>
</table>
3. **QUALITATIVE DATA**

3.1 **NUCLEAR MAGNETIC RESONANCE**

*Sample Preparation:* Dilute analyte to ~10 mg/mL in CDCl₃ containing TMS for 0 ppm reference and dimethylsulfone as quantitative internal standard.

**Instrument:** 400 MHz NMR spectrometer  
**Parameters:**  
Spectral width: at least containing -3 ppm through 13 ppm  
Pulse angle: 90°  
Delay between pulses: 45 seconds

¹H NMR: 5-Fluoro MN-18 Lot# 0468172-5; CDCl₃; 400MHz
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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL into chloroform.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 μm
Carrier Gas: Helium at 1 mL/min
Temperatures: Injector: 280°C
MSD transfer line: 280°C
MS Source: 230°C
MS Quad: 150°C
Oven program:
1) 100°C initial temperature for 1.0 min
2) Ramp to 300°C at 12 °C/min
3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 20:1, 1 μL injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan

Retention Time:

El Mass Spectrum: 5-Fluoro MN-18 Lot# 0468172-5

Latest Revision: 10/13/2016
SWGDRUG.org/monographs.htm
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters:
- Number of scans: 32
- Number of background scans: 32
- Resolution: 4 cm⁻¹
- Sample gain: 8
- Aperture: 150

FTIR ATR (Diamond, 3 Bounce): 5-Fluoro MN-18 Lot# 0468172-5
4. ADDITIONAL RESOURCES

No additional resources as of 10/13/16