1. GENERAL INFORMATION

**IUPAC Name:** N-(naphthalen-1-yl)-1-pentyl-1\textsubscript{H}-indazole-3-carboxamide

**CAS#:** 1391484-80-2

**Synonyms:** NNEI indazole analog

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV\textsubscript{max}(nm):** Not determined

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\textsubscript{23}H\textsubscript{23}N\textsubscript{3}O</td>
<td>357</td>
<td>70.5</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 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

$^1$HNMR: MN-18; Lot# 0451967-39; CDCl₃; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~5 mg/mL in MeOH

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-1 MS (or equivalent); 30m x 0.25 mm x 0.25 µm
Carrier Gas: Helium at 1.0 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: 150
- Tune file: stune.u
- Acquisition mode: scan

Retention Time: 22.724 min

EI Mass Spectrum: MN-18; Lot# 0451967-39
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)
Scan Parameters:
- Number of scans: 32
- Number of background scans: 32
- Resolution: 4 cm\(^{-1}\)
- Sample gain: 8
- Aperture: 150

FTIR ATR (Diamond 1 Bounce): MN-18; Lot# 0451967-39
4. ADDITIONAL RESOURCES

Wikipedia

Forendex