MAB-CHMINACA

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

1. GENERAL INFORMATION

IUPAC Name: \( N\)-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-(cyclohexylmethyl)-1\(H\)-indazole-3-carboxamide

CAS#: 1185887-13-1

Synonyms: ADB-CHMINACA

Source: DEA Reference Material Collection

Appearance: White powder

\(\text{UV}_{\text{max}}(\text{nm})\): 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>(\text{C}<em>{21}\text{H}</em>{30}\text{N}<em>{4}\text{O}</em>{2})</td>
<td>370</td>
<td>141.5</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in DMSO-$d_6$ containing TMS for 0 ppm reference and dimethylfumarate 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: MAB-CHMINACA; Lot# 0466513-1; DMSO-$d_6$; 400MHz

![NMR Spectrogram](image-url)
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~5 mg/mL in CHCl₃

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 µm
Carrier Gas: Helium at 0.6 mL/min
Temperatures:
   - Injector: 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 = 25:1
   - 1 µL injected
MS Parameters:
   - Mass scan range: 30-550 amu
   - Threshold: 150
   - Tune file: stune.u
   - Acquisition mode: scan
Retention Time: 20.35 min

EI Mass Spectrum: MAB-CHMINACA; Lot# 0466513-1
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): MAB-CHMINACA; Lot# 0466513-1
4. ADDITIONAL RESOURCES

Wikipedia

Forendex