Cathine

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

1. GENERAL INFORMATION

IUPAC Name: (1S,2S)-2-amino-1-phenylpropan-1-ol

CAS #: 492-39-7

Synonyms: (+)-norpseudoephedrine; pseudonorephedrine

Source: DEA Reference Material Collection

Appearance: Off-white powder (HCl)

UV$_{max}$: 210 nm

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$<em>9$H$</em>{13}$NO</td>
<td>151</td>
<td>76.3</td>
</tr>
<tr>
<td>HCl</td>
<td>C$<em>9$H$</em>{13}$NO·HCl</td>
<td>187</td>
<td>181.3</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CD$_3$OD

Solvent: Sample diluted to ~10 mg/mL in deuterated methanol (CD$_3$OD) containing TMS for 0 ppm reference and maleic acid as quantitative ISTD

Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

Parameters:
- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle: 90°
- Delay between pulses: 45 seconds
- Number of scans (NT): 8
- Number of steady state scans: 0
- Oversampling: 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

1H NMR: Cathine Lot # N11-P17 CD$_3$OD, 400MHz
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1H NMR: Cathine Lot # N11-P17 CD$_3$OD, 400MHz

Chemical Shift (ppm):
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL in CHCl₃.

Instrument: Gas chromatograph operated in split mode with MS detector

Column: DB-1 MS or equivalent; 30m x 0.25mm x 0.25µm

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 = 25:1, 1 µL injected

MS Parameters:
- Mass scan range: 34-550 amu
- Threshold: 100
- Tune file: stune.u
- Acquisition mode: scan

Retention Time: 5.87 minutes

EI Mass Spectrum: Cathine HCl, Lot # 284
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: 4cm⁻¹
- Sample gain: 8
- Aperture: 150
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FTIR (Diamond ATR, 3 Bounce): Cathine HCl Lot # 284

4. ADDITIONAL RESOURCES

Wikipedia

Forendex