1. GENERAL INFORMATION

**IUPAC Name:** 2-(2,5-dimethoxyphenyl)ethanamine

**CAS #:** 3600-86-0

**Synonyms:** 2,5-dimethoxyphenethylamine

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**Retention Index:** Pending

**UV max:** 225.0, 288.7 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_{10}H_{15}NO_{2}</td>
<td>181</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C_{10}H_{15}NO_{2} \cdot HCl</td>
<td>217</td>
<td>138.9</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D₂O

Sample Preparation: Dilute analyte to ~20 mg/mL in D₂O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

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: 2C-H HCl Lot # MP137-139, D₂O, 400MHz
The Drug Enforcement Administration’s Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

1H NMR: 2C-H HCl Lot # MP137-139, D$_2$O, 400MHz

1H NMR: 2C-H HCl Lot # MP137-139, D$_2$O, 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: DB-1 MS; 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 = 20:1, 1 µL injected

MS Parameters:
- Mass scan range: 30-550 amu
- Threshold: 100
- Tune file: stune.u
- Acquisition mode: scan

Retention Time: 8.036 minutes

EI Mass Spectrum: 2C-H HCl Lot # MP137-139
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

FTIR ATR (Diamond, 3 Bounce): 2C-H HCl Lot # MP137-139
4. ADDITIONAL RESOURCES

Forendex

Wikipedia