5-Iodo-2-aminindan

1. GENERAL INFORMATION

**IUPAC Name:** 5-iodo-2,3-dihydro-1H-inden-2-amine

**CFR:** Not Scheduled (7/2013)

**CAS#:** 132367-76-1

**Synonyms:** 5IAI; 5-IAI; 2,3-dihydro-5-iodo-1H-inden-2-amine

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**Kovat's Index:** Pending

**UV$_{\text{max}}$(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 ($^\circ$C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C$<em>9$H$</em>{10}$IN</td>
<td>259</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C$<em>9$H$</em>{10}$IN·HCl</td>
<td>295</td>
<td>299-301</td>
</tr>
</tbody>
</table>

3. ADDITIONAL RESOURCES

*Forendex*

*Wikipedia*
4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D₂O

*Sample Preparation:* Dilute analyte to ~5 mg/mL in D₂O containing TSP for 0 ppm reference and maleic acid 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

\(^1\)H NMR: 5-iodo-2-aminoindan HCl Lot N17-P44A; D₂O; 400MHz
4.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~1 mg/mL base extracted 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: 8.932 min

EI Mass Spectrum: 5-iodo-2-aminoindan HCl Lot N17-P44A
4.3 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-iodo-2-aminoindan HCl Lot N17-P44A