1. GENERAL INFORMATION

IUPAC Name: 4-methylhexan-2-amine

CFR: Not Scheduled (4/2013)

CAS #: 105-41-9

Synonyms: 1,3-dimethylamylamine, methylhexanamine, 2-amino-4-methylhexane, 1,3-dimethylpentylamine, 4-methyl-2-hexylamine

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

Kovat’s Index: Pending

UV\textsubscript{max}: 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{7}H\textsubscript{17}N</td>
<td>115</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C\textsubscript{7}H\textsubscript{17}N HCl</td>
<td>151</td>
<td>122.9</td>
</tr>
</tbody>
</table>
3. ADDITIONAL RESOURCES

Wikipedia

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR Dimethylfumarate/DMSO

Sample Preparation: Dilute analyte to \(~10 \text{ mg/mL}\) in DMSO 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

![1H NMR: DMAA HCl Lot N1P7; DMSO; 400MHz](image)
**NMR Analytical Observation**

DMAA has two chiral carbons; therefore, two diastereomers are possible. Diastereomers produce slightly different chemical shifts for proton and carbon. Both diastereomers are present in the above spectra.
4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte to ~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 .25mm x .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:** 2.100 minutes

**El Mass Spectrum:** DMAA HCl Lot N1P7
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: 4cm\(^{-1}\)
- Sample gain: 8
- Aperture: 150

FTIR ATR (Diamond, 3 Bounce): DMAA HCl Lot N1P7