1. GENERAL INFORMATION

**IUPAC Name:** 1-(4-chlorobenzamidomethyl)-cyclohexyldimethylamine; hydrochloride

**CAS#:** 1225333-02-7; 41805-00-9 (base)

**Synonyms:** A02

**Source:** Synthesized Material Lot# JLK008-107-02

**Appearance:** White Crystals (HCl)

**UV$_{max}$ (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>HCl</td>
<td>C$<em>{16}$H$</em>{23}$ClN$_{2}$O-HCl</td>
<td>331.28</td>
<td>197.0 ± 2.37</td>
</tr>
<tr>
<td>base</td>
<td>C$<em>{16}$H$</em>{23}$ClN$_{2}$O</td>
<td>294.82</td>
<td>Not determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in deuterated chloroform: methanol (CDCl₃:CD₃OD; 1:5) + TMS.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: 6410.3 Hz containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 30 seconds

¹H NMR: AH-8529 HCl; Lot JLK008-107-02; CDCl₃:CD₃OD (1:5) + TMS; 400 MHz
AH-8529 hydrochloride

The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material.
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~ 1 mg/mL in methanol

Instrument: Shimadzu gas chromatograph operated in split mode with MS detector
Column: Rtx5MS (a DB-5 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: 200°C
Oven program:
1) 90°C initial temperature for 2.0 min
2) Ramp to 300°C at 14°C/min
3) Hold final temperature for 10.0 min

Injection Parameters: Split Ratio = 1:15, 1 μL injected
MS Parameters:
- Mass scan range: 34-550 amu
- Threshold: 100
- Tune file: 050218_Tune.qgt
- Acquisition mode: scan

Retention Time: 15.97 min

EI Mass Spectrum: AH-8529 HCl; Lot JLK008-107-02

Chemical Formula: C_{16}H_{24}ClN_{2}O_{4}^{+}
Exact Mass: 295.15717
AH-8529 hydrochloride

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Zoomed view (126.15 has relative intensity of 100% and is truncated in this view)
3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:**
FTIR with ZnSe ATR attachment (1 bounce)

**Scan Parameters:**
- Number of scans: 4
- Number of background scans: 4
- Resolution: 4 cm\(^{-1}\)
- Sample gain: 8
- Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): AH-8529 HCl; Lot JLK008-107-02

![FTIR Spectrogram](image-url)
AH-8529 hydrochloride

The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material.
AH-8529 hydrochloride

The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material

3.4 RAMAN SPECTROSCOPY

Instrument: Rigaku Progeny 1064
Scan Parameters: Power (mW): 350
Exposure (ms): 1000
Averages: 30
Threshold: 0.80

Raman (1064 nm): AH-8529 HCl; Lot JLK008-107-02
4. ADDITIONAL RESOURCES

1-(3,4-DICHLOROBENZAMIDOMETHYL)CYCLOHEXYLDIMETHYLAMINE
Norman James Harper and George Bryan Austin Veitch

1-(3,4-Dichlorobenzamidomethyl)cyclohexyldimethylamine and related compounds as potential analgesics
N. J. Harper, G. B. A. Veitch, and D. G. Wibberley
Journal of Medicinal Chemistry 1974 17 (11), 1188-1193
DOI: 10.1021/jm00257a012


5. ACKNOWLEDGEMENT

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