3,4-Dichloroethcathinone (DCEC)

Sample Type: Seized Material

Latest Revision: May 18th, 2018
Date Received: January 25th, 2018
Date of Report: May 4th, 2018

1. GENERAL INFORMATION

IUPAC Name: 1-(3,4-dichlorophenyl)-2-(ethylamino)propan-1-one

InChI String: InChI=1S/C11H13Cl2NO/c1-3-14-7(2)11(15)8-4-5-9(12)10(13)6-8/h4-7,14H,3H2,1-2H3

CFR: Not Scheduled (05/2018)

CAS#: Not Available

Synonyms: 3,4-DCEC, DCEC

Source: Department of Homeland Security

Appearance: White Solid Material

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Molecular Ion [M⁺]</th>
<th>Exact Mass [M+H]⁺</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C₁₁H₁₃Cl₂NO</td>
<td>246.1</td>
<td>245</td>
<td>246.0447</td>
</tr>
</tbody>
</table>

Important Note: All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF, and NMR), as no standard reference material was available at the time of testing.

Prepared By: Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT
3. BRIEF DESCRIPTION

3,4-Dichloroethcathinone (DCEC) is classified as a substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Substituted cathinones have been reported to cause stimulant-like effects, similar to amphetamines, which are structurally related to substituted cathinones. Substituted cathinones have also caused adverse events, including deaths, as described in the literature. Structurally similar compounds include cathinone, mephedrone (4-methylmethcathinone), 4-methylethcathinone (4-MEC), ethcathinone (ETH-CAT), and N,N-diethylcathinone. Cathinone, mephedrone, and 4-MEC are all explicitly Schedule I substances in the United States, while ethcathinone is listed as a mephedrone isomer.

4. ADDITIONAL RESOURCES

No additional resources available at this time.

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: NMS Labs (Willow Grove, PA)
Sample Preparation: Acid/Base extraction
Instrument: Agilent 5975 Series GC/MSD System
Column: Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)
Carrier Gas: Helium (Flow: 1.46 mL/min)
Temperatures: Injection Port: 265 °C
Transfer Line: 300 °C
MS Source: 230 °C
MS Quad: 150 °C
Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min
Injection Parameters: Injection Type: Splitless
Injection Volume: 1 µL
MS Parameters:  
Mass Scan Range: 40-550 m/z  
Threshold: 250  
Retention Time: 4.753 min

Chromatogram: 3,4-Dichloroethcathinone

Additional peaks present in chromatogram: internal standard 1 (3.134 min), internal standard 2 (5.770 min)
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 3,4-Dichloroethcathinone
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: 1:100 dilution of acid/base extraction in mobile phase

Instrument: Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC

Column: Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)

Mobile Phase: A: Ammonium formate (10 mM, pH 3.0)

B: Methanol/acetonitrile (50:50)

Flow rate: 0.4 mL/min

Gradient: Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min

Temperatures: Autosampler: 15 °C

Column Oven: 30 °C

Source Heater: 600 °C

Injection Parameters: Injection Volume: 10 µL

QTOF Parameters: TOF MS Scan Range: 100-510 Da

Precursor Isolation: SWATH® acquisition (27 windows)

Fragmentation: Collison Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 5.81 min
Chromatogram: 3,4-Dichloroethcathinone

Additional peaks present in chromatogram: internal standard 1 (4.96 min), internal standard 2 (7.28 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: 3,4-Dichloroethcathinone
5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Dilute powder in DMSO

Instrument: 300 MHz INOVA VARIAN Spectrometer

Parameters: Pulse Sequence: Proton

Solvent: DMSO

Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D

Delay between pulses: 1st delay, d1 = 1.000

1H NMR: 3,4-Dichloroethcathinone
gCOSY NMR: 3,4-Dichloroethcathinone

6. REVISION HISTORY

<table>
<thead>
<tr>
<th>Date</th>
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<tr>
<td>05/18/2018</td>
<td>Added “Sample Type: Seized Material” to Page 1.</td>
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