ANALYTICAL REPORT

Ketamine-Related-Compound-A (C13H16CINO)

1-[(2-chlorophenyl)(methylimino)methyl]cyclopentan-1-ol

Remark – other active cpd. detected: none

Sample ID: 1601-16
Sample description: powder - light yellow
Sample type: RM-reference material
Comments¹: U.S.Pharmacopeia Lot#F0C118; RESPONSE -purchasing
Date of entry: 8/10/2016

Substance identified-structure² (base form)

Systematic name: 1-[(2-chlorophenyl)(methylimino)methyl]cyclopentan-1-ol
Other names: 1-[(2-Chlorophenyl)(methylimino)methyl]cyclopentanol
Formula (per base form) C13H16CINO
Mw (g/mol) 237.73
Salt form: base
StdInChIKey FJGPXUPMNZOTLX-UHFFFAOYSA-N
Compound Class Arylcyclohexylamines
Other active cpd. detected none
Add.info (purity..) pure by HPLC-TOF, impurity detected by GC-MS (possibly thermal degradation byproduct cca 3%)

¹ This report has been produced with the financial support of the Prevention of and Fight against Crime Programme of the European Union (grant agreement number JUST/2013/ISEC/DRUGS/AG/6413). The contents of this report are the sole responsibility of the National Forensic Laboratory and can in no way be taken to reflect the views of the European Commission.
² Created by OPSIN free tool: http://opsin.ch.cam.ac.uk/ DOI: 10.1021/ci100384d
Report updates

<table>
<thead>
<tr>
<th>date</th>
<th>comments (explanation)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Supporting information

Analytical technique: | applied | remarks |
---------------------|---------|---------|
GC-MS (EI ionization)| +       |NFL GC-RT (min): 5,51 BP(1): 152; BP(2): 154, BP(3): 138, |
FTIR-ATR             | +       | direct measurement |
GC-IR (condensed phase)| -       | always as base form |

1. **GC-MS** (Agilent): GC-method is RT locked to tetracosane (9.258 min). Injection volume 1 ml and split mode (1:50). Injector temperature: 280 °C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 190 °C at rate 8 °C/min, then heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, then heating at 50 °C/min up to 325 °C and finally 6.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235 °C, source and quadrupole temperatures 280 °C and 180 °C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300 until 6 min) amu.

2. **FTIR-ATR** (Perkin Elmer): scan range 4000-400 cm⁻¹; resolution 4 cm⁻¹

3. **GC-(MS)-IR** condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny))

GC-method: Injection volume 1 ml and split mode (1:5). Injector temperature 280 °C. Chromatographic separation as above (1). Split MS : IR = 1 : 9. MSD source EI = 70 eV. GC-MS transfer line T= 235 °C, source and quadrupole temperatures 280 °C and 180 °C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu. IR (condensed (solid) phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.
FTIR-ATR

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ketamine Related Compound A_1601-16_UPS1-A</td>
<td>ID: 1601-16-1-(2-Chlorophenyl)((methyl)(methyl)(cyclohexyl)methyloxy)methanone, Lot#FD011B</td>
</tr>
</tbody>
</table>