ANALYTICAL REPORT

3,4-MDPV (C16H21NO3)

1-(2H-1,3-benzodioxol-5-yl)-2-(pyrrolidin-1-yl)pentan-1-one

Remark – other active cpd. detected: none

Sample ID: 1329-16
Sample description: powder - white
Sample type: RM-reference material
Comments¹: Lipomed #1340.1B2.1; RESPONSE -purchasing
Date of entry: 3/11/2016

Substance identified-structure² (base form)

Systematic name: 1-(2H-1,3-benzodioxol-5-yl)-2-(pyrrolidin-1-yl)pentan-1-one
Other names: 3,4-methylenedioxy pyrovalerone
Formula (per base form) C16H21NO3
M_w (g/mol) 275.35
Salt form: HCl
StdInChIKey SYHGEUNFJIGTRX-UHFFFAOYSA-N
Compound Class Cathinones
Other active cpd. detected none
Add.info (purity..) >98.5% (as HCl)

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>
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Supporting information

<table>
<thead>
<tr>
<th>Analytical technique:</th>
<th>applied</th>
<th>remarks</th>
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<tbody>
<tr>
<td>GC-MS (EI ionization)</td>
<td>+</td>
<td>NFL GC-RT (min): 7.91 BP(1): 126; BP(2): 127, BP(3): 149,</td>
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<td>FTIR-ATR</td>
<td>+</td>
<td>direct measurement</td>
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<tr>
<td>GC-IR (condensed phase)</td>
<td>+</td>
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**GC-MS (Agilent):**
- GC-method is RT locked to tetracosane (RT=9.53 min).
- Injection volume 1 ml and split mode (1:50).
- Injector temperature: 280 °C.
- Chromatographic separation
  - Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm.
  - Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, than heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.
  - MSD source EI = 70 eV. GC-MS transfer line T= 235 °C, source and quadropole temperatures 280 °C and 180 °C, respectively.
- Scan range m/z scan range: from 50 (30 until 6 min) to 550 (300) amu.

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

**GC-MS-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny))**
- IR scan range 4000 to 700, resolution 4 cm⁻¹
- GC-method:
  - Injection volume 1 ml and split mode (1:5).
  - Injector temperature: 280 °C.
- Chromatographic separation
  - Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm.
  - Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, than heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.
  - 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 phase) : IR scan range 4000 to 700, resolution 4 cm⁻¹
FIGURES OF SPECTRA

MS (EI)

Abundance

Scan 1591 (7.511 min), 2'-Methylendoxyprovalerone-HCl_1329-16_LIP.D\data.ms

m/z→

0 50000 100000 150000 200000 250000 300000 350000 400000 450000 500000 600000 700000 800000 900000 950000

65.1 96.1 149.0 177.0 204.1 232.1 257.1 274.0