ANALYTICAL REPORT

2-Isovaleryl-1,3-indanedione (C14H14O3)

2-isovalerylindan-1,3-dione

Remark – other active cpd. detected: none

Sample ID: 1600-16
Sample description: powder - yellow
Sample type: RM-reference material
Comments: Dr. Ehren. Lot#50211; RESPONSE -purchasing
Date of entry: 7/18/2016

Substance identified-structure (base form)

Systematic name: 2-isovalerylindan-1,3-dione

Other names: 2-(3-methylbutanoyl)-1H-indene-1,3(2H)-dione;
2-(3-methyl-1-oxobutyl)-1H-indene-1,3(2H)-dione;
Valone;
Isoval;
2-Isovaleryl-1,3-indanedione;
Isovaleryl indandione;
2-Isovaleryl-1,3-indandione

Formula (per base form) C14H14O3
M_w (g/mol) 230.26
Salt form: base
StdInChIKey PVWMAOFPFDINGAY-UHFFFAOYSA-N
Compound Class Others
Other active cpd. detected none

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
Add.info (purity..) | 98 %
---|---

**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): 6.06; BP(1): 173; BP(2): 174; BP(3): 146,</td>
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<tr>
<td>FTIR-ATR</td>
<td>+</td>
<td>direct measurement</td>
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<tr>
<td>GC-IR (condensed phase)</td>
<td>+</td>
<td>always as base form</td>
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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 thickness 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 quadropole 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))
   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 until 6 min.) amu.
   IR (condesed (solid) phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.
FIGURES OF SPECTRA

MS (EI)

Abundance

Scan 1268 (6.062 min): 2-Isovaleryl-1,3-Indanedione_1600-16_DrE_D\data.ms

m/z→

173.1

63.1

89.1

105.1

129.1

146.1

188.1

215.1

230.1