ISONONANOYL CHLORIDE

Molecular formula: \( \text{C}_9\text{H}_{17}\text{ClO} \)
Molecular weight: 176.7
CAS number: 36727-29-4
EC number: 253-168-4

SYNONYM
3,5,5-trimethylhexanoyl chloride

APPEARANCE
Clear liquid with pungent odor.

PHYSICAL PROPERTIES
Density (20 °C): 0.94 g/cm³
Boiling point: 190 °C/101 kPa
Solubility:
Soluble in usual organic solvents (acetone, chloroform, toluene, THF).

CHEMICAL PROPERTIES
- Reacts by hydrolysis yielding hydrochloric acid and isononanoic acid.
- Reacts with amines yielding amides.
- Reacts with alcohols yielding esters.

USES
- Intermediate for organic synthesis.
- Synthesis intermediate for polymerization initiators.
ISONONANOYL CHLORIDE
INCL

### SPECIFICATION

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Guaranteed value</th>
<th>Method</th>
<th>Operating procedure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>Clear liquid</td>
<td>Visual</td>
<td></td>
</tr>
<tr>
<td>Color</td>
<td>≤ 30 APHA</td>
<td>Colorimetry</td>
<td>C – 210</td>
</tr>
<tr>
<td>Total C₈ chlorides</td>
<td>≥ 98.0 %</td>
<td>Gas chromatography</td>
<td>GC – 421</td>
</tr>
<tr>
<td>3,5,5-trimethylhexanoyl chloride</td>
<td>≥ 96.0 %</td>
<td>Gas chromatography</td>
<td>GC – 421</td>
</tr>
<tr>
<td>Alpha ramified chlorides</td>
<td>≤ 2.0 %</td>
<td>Gas chromatography</td>
<td>GC – 421</td>
</tr>
<tr>
<td>Phosgene</td>
<td>≤ 0.05 %</td>
<td>Iodometry</td>
<td>I – 230</td>
</tr>
<tr>
<td>Hydrogen chloride</td>
<td>≤ 0.1 %</td>
<td>Acidimetry</td>
<td>A – 220</td>
</tr>
<tr>
<td>Isononanoic acid</td>
<td>≤ 0.1 %</td>
<td>Gas chromatography</td>
<td>GC – 421</td>
</tr>
<tr>
<td>Isononanoic anhydride</td>
<td>≤ 1.0 %</td>
<td>Gas chromatography</td>
<td>GC – 421</td>
</tr>
<tr>
<td>Carbon tetrachloride</td>
<td>≤ 0.03 %</td>
<td>Gas chromatography</td>
<td>GC – 421</td>
</tr>
<tr>
<td>2-Ethylhexanoyl chloride</td>
<td>≤ 0.15 %</td>
<td>Gas chromatography</td>
<td>GC – 421</td>
</tr>
</tbody>
</table>

### PACKAGING
Polyethylene lined metal drum containing 180 kg.
Polyethylene drum containing 195 kg.
In bulk.

### HANDLING PRECAUTIONS

- **Physicochemical hazard:**
  Flash point (closed cup): 79 °C

- **Health hazards:**
  LD 50 (oral, rat): 1700 mg/kg
  LC 50 (inhalation, rat): 0.06-0.1mg/l/1h
  Irritating on skin, mucous membrane and eyes.
  Corrosive.

- **Recommended:**
  Avoid contact with alkaline products. Wear gloves, goggles, mask and protective clothes.
  If eyes are contaminated wash immediately with clean water for at least 15 minutes.

  If concentrated vapors are inhaled carry person into fresh air.
  In both cases call a physician.

- **Neutralization:**
  Neutralize by reaction with an alkaline solution.

### STORAGE
Stored in its closed original drum in a covered, dry, cool and well-ventilated warehouse the product is stable.

However, in case of prolonged storage it is recommended to check again the product before use by measuring typical parameters of its quality such as color, hydrogen chloride, isononanoic acid and anhydride levels.

### TRANSPORTATION
Refer to MSDS.

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