1. IDENTIFICATION OF THE SUBSTANCE/PREPARATION AND OF THE COMPANY/UNDERTAKING

Identification of the substance/preparation

**Isononanoic acid**

CAS-No: 3302-10-1
EINECS-No: 221-975-0
Use of the Substance/Preparation: Intermediate.

Company/Undertaking Identification

OXEA Deutschland GmbH
Otto-Roelen-Str. 3
D-46147 Oberhausen
Germany

Product Information

Product Stewardship
FAX: +49 (0)208 693 2053
email: psq@oxea-chemicals.com

Emergency telephone number

+49 (0)208 693 2310

2. HAZARDS IDENTIFICATION

Basis for Classification

The product is classified in accordance with Annex VI to Directive 67/548/EEC

Symbol(s)

Xn - Harmful

R-phrase(s)

R22 - Harmful if swallowed
R36/38 - Irritating to eyes and skin

3. COMPOSITION/INFORMATION ON INGREDIENTS

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No</th>
<th>EC No.</th>
<th>Classification</th>
<th>Concentration (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3,5,5-Trimethylhexanoic acid</td>
<td>3302-10-1</td>
<td>221-975-0</td>
<td>Xn;R22</td>
<td>88 - 100</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Xi;R36/38</td>
<td></td>
</tr>
<tr>
<td>6,6-Dimethylheptanoic acid</td>
<td>15898-92-7</td>
<td>none</td>
<td>-</td>
<td>&lt; 1.0</td>
</tr>
<tr>
<td>4,5,5-Trimethylhexanoic acid</td>
<td>94349-37-8</td>
<td>none</td>
<td>-</td>
<td>&lt; 2.0</td>
</tr>
<tr>
<td>2,5,5-Trimethylhexanoic acid</td>
<td>53705-45-6</td>
<td>none</td>
<td>-</td>
<td>&lt;= 1.0</td>
</tr>
</tbody>
</table>

Remarks

Mixture of isomeric Isononanoic acids, mainly 3,5,5-Trimethylhexanoic acid.

4. FIRST AID MEASURES
4. FIRST AID MEASURES

General advice
Remove contaminated, soaked clothing immediately and dispose of safely.

Inhalation
Keep at rest. Aerate with fresh air. When symptoms persist or in all cases of doubt seek medical advice.

Eyes
Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Remove contact lenses. Immediate medical attention is required.

Skin
Wash off immediately with soap and plenty of water. When symptoms persist or in all cases of doubt seek medical advice.

Ingestion
Call a physician immediately. Do not induce vomiting without medical advice.

Special hazard
Lung irritation.

Notes to physician
Treat symptomatically. If ingested, flush stomach and compensate acidosis.

5. FIRE-FIGHTING MEASURES

Suitable extinguishing media
foam, dry chemical, carbon dioxide (CO2)

Extinguishing media which must not be used for safety reasons
Do not use a solid water stream as it may scatter and spread fire.

Special exposure hazards arising from the substance or preparation itself, its combustion products, or released gases
Under conditions giving incomplete combustion, hazardous gases produced may consist of:
carbon monoxide (CO)
carbon dioxide (CO2)
Combustion gases of organic materials must in principle be graded as inhalation poisons

Special protective equipment for fire-fighters
Firefighter protection should include a self-contained breathing apparatus (NIOSH-approved or EN 133) and full firefighting turn out gear.

Precautions for fire-fighting
Cool containers / tanks with water spray. Water run-off and vapor cloud may be corrosive. Dike and collect water used to fight fire. Keep people away from and upwind of fire.

6. ACCIDENTAL RELEASE MEASURES
6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Avoid contact with skin and eyes. Avoid breathing vapors or mists. Keep people away from and upwind of spill/leak. Ensure adequate ventilation, especially in confined areas. Keep away from heat and sources of ignition. For personal protection see section 8.

Environmental precautions
Prevent further leakage or spillage. Do not discharge product into the aquatic environment without pretreatment (biological treatment plant).

Methods for containment
Stop the flow of material, if possible without risk. Dike spilled material, where this is possible.

Methods for cleaning up
Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. If liquid has been spilt in large quantities clean up promptly by scoop or vacuum. Dispose of in accordance with local regulations.

7. HANDLING AND STORAGE

Handling
Advice on safe handling
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product. Provide sufficient air exchange and/or exhaust in work rooms.

Advice on protection against fire and explosion
Keep away from sources of ignition - No smoking. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours). In case of fire, emergency cooling with water spray should be available. Ground and bond containers when transferring material.

Storage
Technical measures/Storage conditions
Keep containers tightly closed in a cool, well-ventilated place. Handle and open container with care.

Suitable material: stainless steel
Unsuitable material: mild steel, copper, brass, including their alloys

Advice on common storage
Incompatible products:
bases
amines

Temperature class
T2

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

Exposure limits European Union
No exposure limits established.

Exposure limits UK
Occupational exposure controls

Engineering measures
General or dilution ventilation is frequently insufficient as the sole means of controlling employee exposure. Local ventilation is usually preferred. Explosion-proof equipment (for example fans, switches, and grounded ducts) should be used in mechanical ventilation systems.

Personal protective equipment

General industrial hygiene practice
Avoid contact with skin, eyes and clothing. Do not breathe vapours or spray mist. Ensure that eyewash stations and safety showers are close to the workstation location.

Hygiene measures
When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

Hand protection
Wear protective gloves. Recommendations are listed below. Other protective material may be used, depending on the situation, if adequate degradation and permeation data is available. If other chemicals are used in conjunction with this chemical, material selection should be based on protection for all chemicals present.

- Suitable material: nitrile rubber
  Evaluation: according to EN 374: level 6
  Glove thickness: approx 0.55 mm
  Break through time: > 480 min

- Suitable material: polyvinylchloride
  Evaluation: Information derived from practical experience
  Glove thickness: approx 0.8 mm

Eye protection
Safety glasses with side-shields. In addition to goggles, wear a face shield if there is a reasonable chance for splash to the face. Equipment should conform to EN 166.

Skin and body protection
Impervious clothing. Wear face-shield and protective suit for abnormal processing problems.

Environmental exposure controls
Exhaust ventilation equipped with scrubbers. Dispose of wastes in an approved waste disposal facility. Inform the responsible authorities in case of gas leakage, or of entry into waterways, soil or drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

<table>
<thead>
<tr>
<th>Physical state</th>
<th>liquid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Colour</td>
<td>colourless</td>
</tr>
<tr>
<td>Odour</td>
<td>slightly acidic</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>158,23</td>
</tr>
</tbody>
</table>
9. PHYSICAL AND CHEMICAL PROPERTIES

Molecular formula C9H18O2

Flash point 120 - 137 °C
  Method EN 22719

Autoignition temperature 320 - 405 °C
  Method DIN 51794

Lower explosion limit 1,2 Vol %

Melting point/range < -60 °C

Boiling point/range 230 - 240 °C @ 1013 hPa

Vapour pressure

Values [hPa] @ °C @ °F
0,01 - 0,04 20 68
0,2 50 122

Density

Values [g/cm³] @ °C @ °F Method
0,899 20 68 DIN 51757
0,876 50 122 DIN 51757

Refractive index 1,429 @ 20 °C

Viscosity 10 - 12 mPa*s @ 20 °C
  Method DIN 51562, dynamic

pH 3,5

Water solubility 0,3 g/l @ 20 °C

log Pow 3,0 (calculated; Leo-Hansch)

10. STABILITY AND REACTIVITY

Stability
Stable under recommended storage conditions.

Conditions to avoid
Avoid contact with heat, sparks, open flame, and static discharge. Avoid any source of ignition.

Materials to avoid
bases, amines.

Hazardous decomposition products
No decomposition if stored and applied as directed.

11. TOXICOLOGICAL INFORMATION

Principle Routes of Exposure Inhalation, Eye contact, Skin contact, Ingestion

Acute toxicity

<table>
<thead>
<tr>
<th>Routes of Exposure</th>
<th>Endpoint</th>
<th>Values</th>
<th>Species</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>3,5,5-Trimethylhexanoic acid (3302-10-1)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Oral LD50 3135 mg/kg rat
Oral LD50 1160 mg/kg rat OECD 401
Dermal LD50 > 2000 mg/kg rat

**Irritation and corrosion**

<table>
<thead>
<tr>
<th>Target Organ Effects</th>
<th>Species</th>
<th>Result</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>3,5,5-Trimethylhexanoic acid (3302-10-1)</td>
<td>Eyes</td>
<td>rabbit</td>
<td>Mild eye irritation</td>
</tr>
<tr>
<td>3,5,5-Trimethylhexanoic acid (3302-10-1)</td>
<td>Eyes</td>
<td>rabbit</td>
<td>severe irritation</td>
</tr>
<tr>
<td>3,5,5-Trimethylhexanoic acid (3302-10-1)</td>
<td>Skin</td>
<td>rabbit</td>
<td>Mild skin irritation</td>
</tr>
<tr>
<td>3,5,5-Trimethylhexanoic acid (3302-10-1)</td>
<td>Skin</td>
<td>rabbit</td>
<td>severe irritation</td>
</tr>
</tbody>
</table>

**Subacute, subchronic and prolonged toxicity**

<table>
<thead>
<tr>
<th>Type</th>
<th>Dose Levels</th>
<th>Species</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oral</td>
<td>NOAEL: 10 mg/kg/d</td>
<td>rat</td>
<td>OECD 407</td>
</tr>
</tbody>
</table>

**Carcinogenicity, Mutagenicity, Reproductive toxicity**

<table>
<thead>
<tr>
<th>Type</th>
<th>Dose Levels</th>
<th>Species</th>
<th>Evaluation</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mutagenicity</td>
<td>Salmonella typhimurium</td>
<td>negative</td>
<td>OECD 471 (Ames)</td>
<td>In vitro study</td>
</tr>
<tr>
<td>Mutagenicity</td>
<td>Escherichia coli</td>
<td>negative</td>
<td>OECD 472</td>
<td>In vitro study</td>
</tr>
</tbody>
</table>

**Note**

Handle in accordance with good industrial hygiene and safety practice.

## 12. ECOLOGICAL INFORMATION

**Acute aquatic toxicity**

<table>
<thead>
<tr>
<th>Species</th>
<th>Exposure time</th>
<th>Dose Levels</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>3,5,5-Trimethylhexanoic acid (3302-10-1)</td>
<td>Lepomis gibbosus (Pumpkinseed sunfish)</td>
<td>96h</td>
<td>LC50: 190 mg/l</td>
</tr>
<tr>
<td>3,5,5-Trimethylhexanoic acid (3302-10-1)</td>
<td>Salmo Gairdneri</td>
<td>96h</td>
<td>LC50: 160 mg/l</td>
</tr>
<tr>
<td>3,5,5-Trimethylhexanoic acid (3302-10-1)</td>
<td>Oncorhynchus mykiss (rainbow trout)</td>
<td>96h</td>
<td>LC50: 122 mg/l</td>
</tr>
<tr>
<td>3,5,5-Trimethylhexanoic acid (3302-10-1)</td>
<td>Activated sludge (bacteria)</td>
<td>3 h</td>
<td>EC50: 470 mg/l</td>
</tr>
</tbody>
</table>

**Biodegradation**

80 % (14 d), activated sludge, industrial, non-adapted, OECD 302 B (Zahn-Wellens Test).

**Note**

Avoid release to the environment.

## 13. DISPOSAL CONSIDERATIONS
13. DISPOSAL CONSIDERATIONS

Product Information
Disposal required in compliance with all waste management related state and local regulations. The choice of the appropriate method of disposal depends on the product composition by the time of disposal as well as the local statutes and possibilities for disposal.

Uncleaned empty packaging
Contaminated packaging should be emptied as far as possible and after appropriate cleansing may be taken for reuse.

14. TRANSPORT INFORMATION

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>ADR/RID</td>
<td>Not restricted</td>
</tr>
<tr>
<td>ADNR</td>
<td>ADNR: Container and Tanker</td>
</tr>
<tr>
<td>ICAO/IATA</td>
<td>Not restricted</td>
</tr>
<tr>
<td>IMDG</td>
<td>Not restricted</td>
</tr>
</tbody>
</table>

15. REGULATORY INFORMATION

Labelling according to EC Directives

Basis for Classification
The product is classified in accordance with Annex VI to Directive 67/548/EEC
contains 3,5,5-Trimethylhexanoic acid (CAS 3302-10-1)

Symbol(s) Xn - Harmful

R-phrase(s) R22 - Harmful if swallowed
R36/38 - Irritating to eyes and skin

S-phrase(s) S26 - In case of contact with eyes, rinse immediately with plenty of water and seek medical advice
S37 - Wear suitable gloves

Water contaminating class (Germany)
Water contaminating class 1
KBwS Number 1277
KBwS Classification Annex 1 or 2

DI 96/82/EC (Seveso II)
Category not subject

Other regulations
International Inventories

3,5,5-Trimethylhexanoic acid, CAS 3302-10-1
   AICS (AU)
   DSN (CA)
   IECSC (CN)
   EC-No. 2219750 (EU)
   ENCS (2)-608 (JP)
   KECI KE-34559 (KR)
   PICCS (PH)
   TSCA (US)

National regulatory information Great Britain

This classification following EG guidelines is also in accordance with the Chemicals (Hazard Information and Packaging for Supply) Regulation CHIP (as amended).

16. OTHER INFORMATION

Full text of R-phrases referred to under sections 2 and 3
R22 - Harmful if swallowed
R36/38 - Irritating to eyes and skin

Revision Date  26-Sep-2008
Issuing date   26-Sep-2008

Training advice
For effective first-aid, special training / education is needed.

Sources of key data used to compile the datasheet
Information contained in this safety data sheet is based on Oxea owned data and public sources deemed valid or acceptable. The absence of data elements required by ANSI or 2001/58/EC indicates, that no data meeting these requirements is available.

Further information for the safety data sheet
Changes against the previous version are marked by ***. Observe national and local legal requirements. For more information, other material safety data sheets or technical data sheets please consult the Oxea homepage (www.oxea-chemicals.com).
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