

Material Safety Data Sheet



10310
Isononanoic acid

Revision Date 26-Sep-2008
Revision Number 1.00

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-phrases)

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

3. COMPOSITION/INFORMATION ON INGREDIENTS

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

Remarks

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

4. FIRST AID MEASURES

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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

Fire fighter protection should include a self-contained breathing apparatus (NIOSH-approved or EN 133) and full fire-fighting 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

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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

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No exposure limits established.

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

Physical state	liquid
Colour	colourless
Odour	slightly acidic
Molecular weight	158,23

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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/cm ³]	@ °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

Routes of Exposure	Endpoint	Values	Species	Method
3,5,5-Trimethylhexanoic acid (3302-10-1)				

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Oral	LD50	3135 mg/kg	rat	
Oral	LD50	1160 mg/kg	rat	OECD 401
Dermal	LD50	> 2000 mg/kg	rat	

Irritation and corrosion

Target Organ Effects	Species	Result	Method	
3,5,5-Trimethylhexanoic acid (3302-10-1)				
Eyes	rabbit	Mild eye irritation	OECD 405	in vivo
Eyes	rabbit	severe irritation		in vivo
Skin	rabbit	Mild skin irritation	OECD 404	in vivo
Skin	rabbit	severe irritation	OECD 404	in vivo

Subacute, subchronic and prolonged toxicity

Type	Dose Levels	Species	Method	
3,5,5-Trimethylhexanoic acid (3302-10-1)				
Oral	NOAEL: 10 mg/kg/d	rat	OECD 407	

Carcinogenicity, Mutagenicity, Reproductive toxicity

Type	Dose Levels	Species	Evaluation	Method	
3,5,5-Trimethylhexanoic acid (3302-10-1)					
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	In vitro study
Mutagenicity		Escherichia coli	negative	OECD 472	In vitro study

Note

Handle in accordance with good industrial hygiene and safety practice.

12. ECOLOGICAL INFORMATION

Acute aquatic toxicity

Species	Exposure time	Dose Levels	Method
3,5,5-Trimethylhexanoic acid (3302-10-1)			
Lepomis gibbosus (Pumpkinseed sunfish)	96h	LC50: 190 mg/l	DIN 38412
Salmo Gairdneri	96h	LC50: 160 mg/l	DIN 38412
Oncorhynchus mykiss (rainbow trout)	96h	LC50: 122 mg/l	OECD 203
Activated sludge (bacteriae)	3 h	EC50: 470 mg/l	OECD 209

3,5,5-Trimethylhexanoic acid, CAS 3302-10-1

Biodegradation

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

Note

Avoid release to the environment.

13. DISPOSAL CONSIDERATIONS

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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

<u>ADR/RID</u>	Not restricted
<u>ADNR</u>	ADNR: Container and Tanker Not restricted
<u>ICAO/IATA</u>	Not restricted
<u>IMDG</u>	Not restricted

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

<u>contains</u>	3,5,5-Trimethylhexanoic acid (CAS 3302-10-1)
<u>Symbol(s)</u>	Xn - Harmful
<u>R-phrases(s)</u>	R22 - Harmful if swallowed R36/38 - Irritating to eyes and skin
<u>S-phrases(s)</u>	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)

<u>Water contaminating class</u>	1
<u>KBwS Number</u>	1277
<u>KBwS Classification</u>	Annex 1 or 2

DI 96/82/EC (Seveso II)

<u>Category</u>	not subject
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Other regulations

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International Inventories

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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

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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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