SAFETY DATA SHEET

Isononanoic acid
10310

Version / Revision	5.01	**Revision Date**	30-Sep-2021
Supersedes Version	5.00***	**Issuing date**	30-Sep-2021

SECTION 1: Identification

1.1. Product identifier

Identification of the substance/preparation **Isononanoic acid**

Chemical Name 3,5,5-Trimethylhexanoic acid
CAS-No 3302-10-1

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the Substance / Preparation Intermediate
lubricant
Uses advised against None

1.3. Details of the supplier of the safety data sheet

Supplier

OQ Chemicals Corporation
15375 Memorial Drive
West Memorial Place I
Suite 300
Houston, TX 77079
USA
Phone +1 346 378 7300

Product Information

Product Stewardship
FAX: +49 (0)208 693 2053
email: sc.psq@oq.com

1.4. Emergency telephone number

Emergency telephone number NCEC +1 202 464 2554
available 24/7

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

This substance is classified in accordance with paragraph (d) of §1910.1200 (GHS-US classification).

Acute oral toxicity Category 4, H302
Skin corrosion/irritation Category 2, H315
Serious eye damage/eye irritation Category 1, H318
Environmental hazard Aquatic Acute 3; H402

OSHA Specified Hazards Not applicable.

2.2. Label elements

Labeling according to §1910.1200 (GHS-US labeling).

Hazard symbol(s)

Signal word **Danger**

Hazard statements
H302: Harmful if swallowed.
H315: Causes skin irritation.
H318: Causes serious eye damage.
H402: Harmful to aquatic life

Precautionary statements

Prevention
P264: Wash hands thoroughly after handling.
P270: Do not eat, drink or smoke when using this product.
P273: Avoid release to the environment.
P280: Wear protective gloves/eye protection/face protection.

Response
P301 + P312: IF SWALLOWED: Call a POISON CENTRE/doctor if you feel unwell.
P330: Rinse mouth.
P302 + P352: IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310: Immediately call a POISON CENTER/doctor.
P362 + P364: Take off contaminated clothing and wash it before reuse.

Disposal
P501: Dispose of contents/container in accordance with local regulation.

2.3. Other hazards

Vapour/air-mixtures are explosive at intense warming

SECTION 3: Composition / information on ingredients

3.1. Substances

Component	CAS-No	Concentration (%)
3,5,5-Trimethylhexanoic acid***	3302-10-1	88,5 - 100

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

SECTION 4: First aid measures

4.1. Description of first aid measures

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

Skin
Wash off immediately with soap and plenty of water. 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.

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

4.2. Most important symptoms and effects, both acute and delayed

Main symptoms
cough, headache, nausea, shortness of breath.

Special hazard
Lung irritation, Lung oedema.

4.3. Indication of any immediate medical attention and special treatment needed

General advice
Remove contaminated, soaked clothing immediately and dispose of safely. First aider needs to protect himself.

Treat symptomatically. If ingested, flush stomach and compensate acidosis.

SECTION 5: Firefighting measures

5.1. Extinguishing media

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

Unsuitable Extinguishing Media
Do not use a solid water stream as it may scatter and spread fire.

5.2. Special hazards arising from the substance or mixture

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
Vapour/air-mixtures are explosive at intense warming
Vapours are heavier than air and may spread along floors

5.3. Advice for firefighters

Special protective equipment for firefighters
Fire fighter protection should include a self-contained breathing apparatus (NIOSH-approved or EN 133) and full fire-fighting turn out gear.

Precautions for firefighting
Cool containers / tanks with water spray. Dike and collect water used to fight fire. Keep people away from and upwind of fire.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel: For personal protective equipment see section 8. 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 emergency responders: Personal protection see section 8.

6.2. Environmental precautions

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

6.3. Methods and material for containment and cleaning up

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. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours).

6.4. Reference to other sections

For personal protective equipment see section 8.

SECTION 7: Handling and storage

7.1. Precautions for safe 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.

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.

Advice on the protection of the environment
See Section 8: Environmental exposure controls.

Incompatible products
bases
amines

7.2. Conditions for safe storage, including any incompatibilities

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. Vapour/air-mixtures are explosive at intense warming.

Technical measures/Storage conditions
Keep containers tightly closed in a cool, well-ventilated place. Handle and open container with care. Keep at temperatures between 0 and 38 °C (32 and 100 °F).

Suitable material
stainless steel

Unsuitable material
mild steel, copper, brass, including their alloys

SECTION 8: Exposure controls / personal protection

8.1. Control parameters

Exposure limits United States of America

No exposure limits established.

8.2. Exposure controls

Appropriate Engineering controls
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.

Individual protection measures, such as 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.

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.

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

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

Respiratory protection
Respirator with filter for organic vapour. Use the indicated respiratory protection if the occupational exposure limit is exceeded and/or in case of product release (vapor or mist). Equipment should conform to NIOSH.

Environmental exposure controls
If possible use in closed systems. If leakage can not be prevented, the substance needs to be suck off at the emersion point, if possible without danger. Observe the exposure limits, clean exhaust air if needed. If recycling is not practicable, dispose of in compliance with local regulations. Inform the responsible authorities in case of leakage into the atmosphere, or of entry into waterways, soil or drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	liquid @ 20 °C (68 °F)
Colour	colourless
Odour	slightly acidic
Odour threshold	No data available
pH	4,4 (0,1 g/l in water @ 25 °C (77 °F)) DIN 19268***

Melting point/range	-106,6 °F (-77 °C) (Pour point)
Method	DIN ISO 3016
Boiling point/range	456,8 °F (236 °C) @ 1 atm (101,3 kPa)
Method	OECD 103
Flash point	242,6 °F (117 °C) @ 1013 hPa***
Method	ISO 2719
Evaporation rate	No data available
Flammability (solid, gas)	Does not apply, the substance is a liquid
Lower explosion limit	1,2 Vol %
Upper explosion limit	No data available

Vapour pressure

Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
0,0046	0,00046	< 0,001	20	68	OECD 104***
4,5	0,45	0,004	50	122	OECD 104***

Vapour density No data available

Relative density

Values	@ °C	@ °F	Method
0,900	20	68	DIN 51757
0,876	50	122	DIN 51757

Solubility	0,7 g/l @ 68 °F (20 °C), water, OECD 105
log Pow	3,2 @ 25 °C (77 °F) measured OECD 117***
Autoignition temperature	779 °F (415 °C) @ 1009 hPa***
Method	DIN 51794
Decomposition temperature	No data available
Viscosity	11,47 mPa*s @ 68 °F (20 °C)
Method	DIN 51562, dynamic

9.2. Other information

Molecular weight	158,23
Molecular formula	C9 H18 O2
log Koc	2,79 @ pH 4,5 1,90 @ pH 8 calculated***
Dissociation constant	pKa 4,8 @ 20 °C (68 °F), OECD 112***
Oxidizing properties	Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties
Refractive Index	1,429 @ 68 °F (20 °C)
Explosive properties	Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties
Surface tension	35,3 mN/m (0,63 g/l @ 20°C (68°F)), OECD 115

SECTION 10: Stability and Reactivity

10.1. Reactivity

The reactivity of the product corresponds to the typical reactivity shown by the substance group as described in any text book on organic chemistry.

10.2. Chemical stability

Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

Hazardous polymerisation does not occur.

10.4. Conditions to avoid

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

10.5. Incompatible materials

bases, amines.

10.6. Hazardous decomposition products

No decomposition if stored and applied as directed.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Likely routes of exposure Ingestion, Inhalation, Eye contact, Skin contact

3,5,5-Trimethylhexanoic acid*, CAS: 3302-10-1**
Main symptoms
cough, headache, nausea, shortness of breath.
Target Organ Systemic Toxicant - Single exposure
Based on available data, the classification criteria are not met for:
STOT SE
Target Organ Systemic Toxicant - Repeated exposure
Based on available data, the classification criteria are not met for:
STOT RE

Acute toxicity				
3,5,5-Trimethylhexanoic acid (3302-10-1)				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	1160 mg/kg	rat, male/female	OECD 401
Dermal	LD50	> 2000 mg/kg	rat, male/female	
Inhalative***	LC0***	0,03 mg/l (7 h)***	rat, male/female***	OECD 403***

3,5,5-Trimethylhexanoic acid*, CAS: 3302-10-1**
Assessment
The available data lead to the classification given in section 2***

Irritation and corrosion

3,5,5-Trimethylhexanoic acid (3302-10-1)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	irritating	OECD 404	4h in vivo***
Eyes	rabbit	severe irritation	OECD 405	72h in vivo***
Respiratory tract***	mouse***	RD50: 420 mg/m³***		in vivo***

3,5,5-Trimethylhexanoic acid*, CAS: 3302-10-1**
Assessment
The available data lead to the classification given in section 2***

Sensitization				
3,5,5-Trimethylhexanoic acid (3302-10-1)				
Target Organ Effects	Species	Evaluation	Method	
Skin	guinea pig	not sensitizing	OECD 406	

3,5,5-Trimethylhexanoic acid*, CAS: 3302-10-1**
Assessment
Based on available data, the classification criteria are not met for:
Skin sensitization
For respiratory sensitization, no data are available

Subacute, subchronic and prolonged toxicity				
3,5,5-Trimethylhexanoic acid (3302-10-1)				
Type	Dose	Species	Method	
Subacute toxicity	NOAEL: 10 mg/kg/d***	rat, male***	OECD 422***	Oral
Subchronic toxicity***	NOAEL: 5 mg/kg/d (90d)***	rat, male/female***	OECD 408***	Oral***

3,5,5-Trimethylhexanoic acid*, CAS: 3302-10-1**
Assessment
Based on available data, the classification criteria are not met for:
STOT RE

Carcinogenicity, Mutagenicity, Reproductive toxicity					
3,5,5-Trimethylhexanoic acid (3302-10-1)					
Type	Dose	Species	Evaluation	Method	
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	In vitro study
Mutagenicity		Escherichia coli	negative	OECD 472	In vitro study
Mutagenicity		human lymphocytes***	negative***	OECD 473 (Chromosomal Aberration)	In vitro study
Mutagenicity		V79 cells, Chinese hamster	negative	OECD 476 (Mammalian Gene Mutation)	In vitro study
Reproductive toxicity	LOAEL 165 - 500 mg/kg/d	rat, parental, female		OECD 415	Oral

Reproductive toxicity	NOAEL 79 - 228 mg/kg/d	rat, parental, female		OECD 415	Oral
Reproductive toxicity***	NOAEL 10 - 30 mg/kg/d***	rat, parental male/female***		OECD 422***	Oral***
Reproductive toxicity***	NOAEL 100 mg/kg/d***	rat, 1. Generation, male/female***		OECD 422***	Oral***
Reproductive toxicity***	NOAEL 120 mg/kg/d***	rat, parental male/female***		OECD 443***	Oral***
Reproductive toxicity***	NOAEL 25 mg/kg/d***	rat, 1. Generation, male/female***		OECD 443***	Oral***
Developmental Toxicity***	NOAEL 60 mg/kg/d***	rat***		OECD 414, Oral***	Maternal toxicity Developmental toxicity***
Developmental Toxicity***	NOAEL 250 mg/kg/d***	rabbit***		OECD 414, Oral***	Maternal toxicity Developmental toxicity***

3,5,5-Trimethylhexanoic acid*, CAS: 3302-10-1**
CMR Classification
The available data on CMR properties are summarized in the table above. They do not indicate a classification into categories 1A or 1B
Evaluation
In vitro tests did not show mutagenic effects

3,5,5-Trimethylhexanoic acid*, CAS: 3302-10-1**
Aspiration toxicity
no data available
Note
Handle in accordance with good industrial hygiene and safety practice. Further details on substance data can be found in the registration dossier under the following link:
http://echa.europa.eu/information-on-chemicals/registered-substances.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity			
3,5,5-Trimethylhexanoic acid (3302-10-1)			
Species	Exposure time	Dose	Method
Oncorhynchus mykiss (rainbow trout)	96h	LC50: 122 mg/l	OECD 203
Activated sludge (bacteriae)	3 h	EC50: 470 mg/l	OECD 209
Daphnia magna (Water flea)	48h	EC50: 68 mg/l	OECD 202
Pseudokirchneriella subcapitata	72h	EC50: 81 mg/l (Growth rate)	OECD 201
Pseudokirchneriella subcapitata	72h	EC50: 51 mg/l (Biomass)	OECD 201

Long term toxicity

3,5,5-Trimethylhexanoic acid (3302-10-1)				
Type	Species	Dose	Method	
Aquatic toxicity	Pseudokirchneriella subcapitata	NOEC: 10 mg/l (3d)***	OECD 201	

12.2. Persistence and degradability

3,5,5-Trimethylhexanoic acid*, CAS: 3302-10-1**
Biodegradation
96 % (21 d), activated sludge, domestic, non-adapted, aerobic, OECD 301A.***

Abiotic Degradation		
3,5,5-Trimethylhexanoic acid (3302-10-1)		
Type	Result	Method
Hydrolysis	not expected***	
Photolysis	Half-life (DT50): 60,17 h***	calculated

12.3. Bioaccumulative potential

3,5,5-Trimethylhexanoic acid (3302-10-1)		
Type	Result	Method
log Pow	3,2 @ 25 °C (77 °F)***	measured, OECD 117
BCF	4,1 - 7 @ 0,1 mg/l	OECD 305 C
BCF	0,5 - 1,7 @ 1 mg/l	OECD 305 C

12.4. Mobility in soil

3,5,5-Trimethylhexanoic acid (3302-10-1)		
Type	Result	Method
Surface tension	35,3 mN/m (0,63 g/l @ 20°C (68°F))	OECD 115
Distribution to environmental compartments	Air: 1,99 Soil: 12,6 Water: 72,6 Sediment: 12,7 Suspended sediment: 0,08 Biota: 0,01***	calculated
Adsorption/Desorption	log Koc: 2,79 @ pH 4,5	calculated
Adsorption/Desorption	log Koc: 1,90 @ pH 8	calculated

12.5. Results of PBT and vPvB assessment

3,5,5-Trimethylhexanoic acid*, CAS: 3302-10-1**
PBT and vPvB assessment
This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)

12.6. Other adverse effects

3,5,5-Trimethylhexanoic acid*, CAS: 3302-10-1**
No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

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.

SECTION 14: Transport information

Section 14.1 - 14.6

D.O.T. (49CFR)	Not restricted
ICAO-TI / IATA-DGR	Not restricted
IMDG	Not restricted

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Product name	Nonanoic acid
Ship type	3
Pollution category	Y

SECTION 15: Regulatory information

Federal and State Regulations
Components of the product are listed in the quoted regulations. For details please refer to the regulations directly. This list is not exhaustive, please check for other applicable regulations.

Federal Regulations
This product is listed on the TSCA inventory

International Inventories

3,5,5-Trimethylhexanoic acid*, CAS: 3302-10-1**
AICS (AU)
DSL (CA)
IECSC (CN)
EC-No. 2219750 (EU)
ENCS (2)-608 (JP)
ISHL (2)-608 (JP)
KECI KE-34559 (KR)
PICCS (PH)
TSCA (US)
NZIoC-NZ with note***
TCSI (TW)

SECTION 16: Other information

Revision Date	30-Sep-2021
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Hazard Rating Systems

NFPA (National Fire Protection Association)

Health Hazard	2
Fire Hazard	1
Reactivity	0

HMIS (Hazardous Material Information System)

Health Hazard	2
Flammability	1
Physical Hazard	0

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 OQ owned data and public sources deemed valid or acceptable. The absence of data elements required by OSHA, ANSI or Annex II, Regulation 1907/2006/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 OQ homepage (www.chemicals.oq.com).
The use of a comma in section 3 and section 7 to 12 is the same as a period.

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End of Safety Data Sheet