

SAFETY DATA SHEET



Isononanol
10320

Version / Revision
Supersedes Version

5.01
5.00***

Revision Date
Issuing date

25-Jan-2022
25-Jan-2022

SECTION 1: Identification

1.1. Product identifier

Identification of the
substance/preparation

Isononanol

Chemical Name
CAS-No

3,5,5-Trimethylhexan-1-ol
3452-97-9

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

Use of the Substance /
Preparation

Intermediate

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).

Skin corrosion/irritation Category 2, H315
Serious eye damage/eye irritation Category 2A, H319
Target Organ Systemic Toxicant - Repeated exposure Category 2, H373
Flammable liquid Category 4, H227

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Environmental hazard Aquatic Acute 2; H401

OSHA Specified Hazards Not applicable.

2.2. Label elements

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

Hazard symbol(s)



Signal word

Warning

Hazard statements

H227: Combustible liquid
H315: Causes skin irritation.
H319: Causes serious eye irritation.
H373: May cause damage to organs through prolonged or repeated exposure if swallowed.
H401: Toxic to aquatic life

Precautionary statements

Prevention

P210: Keep away from flames and hot surfaces. - No smoking.
P280: Wear protective gloves/eye protection/face protection.
P264: Wash hands thoroughly after handling.
P260: Do not breathe gas/mist/vapours.
P273: Avoid release to the environment.

Response

P302 + P352: IF ON SKIN: Wash with plenty of water.
P332 + P313: If skin irritation occurs: Get medical advice/ attention.
P362 + P364: Take off contaminated clothing and wash it before reuse.
P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313: If eye irritation persists: Get medical advice/ attention.
P314: Get medical advice/attention if you feel unwell.

Storage

P403 + P235: Store in a well ventilated place. Keep cool.

Disposal

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

2.3. Other hazards

Components of the product may be absorbed into the body by inhalation, ingestion and through the skin

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Vapour/air-mixtures are explosive at intense warming

SECTION 3: Composition / information on ingredients

3.1. Substances

Component	CAS-No	Concentration (%)
3,5,5-Trimethylhexan-1-ol	3452-97-9	> 97,5

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 plenty of water for at least 15 minutes. 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, nausea, gastrointestinal discomfort, vomiting.

Special hazard

Lung irritation, Liver effects, Kidney disorders.

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, irrigate the stomach using activated charcoal.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

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alcohol-resistant 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

Vapours are heavier than air and may spread along floors

Vapour/air-mixtures are explosive at intense warming

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

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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

strong acids
strong oxidizing agents

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.

SECTION 8: Exposure controls / personal protection

8.1. Control parameters

Exposure limits United States of America

No exposure limits established regarding ACGIH, OSHA Z-1 and OSHA Z-2.

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.

Engineering and risk Management measures should maintain strictly controlled conditions. This also applies to environmental exposure controls.

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Individual protection measures, such as personal protective equipment

General industrial hygiene practice

Avoid contact with skin, eyes and clothing. Do not breathe dust or 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

Tightly fitting safety goggles. 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
Reference substance	2-Ethylhexanol
Evaluation	according to EN 374: level 6
Glove thickness	approx 0,55 mm
Break through time	> 480 min

Suitable material	polyvinylchloride / nitrile rubber
Reference substance	2-Ethylhexanol
Evaluation	according to EN 374: level 6
Glove thickness	approx 0,9 mm
Break through time	> 480 min

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. 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

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Colour colourless
Odour alcoholic
Odour threshold No data available
pH No data available
Melting point/range -112 °F (-80 °C) @ 1013 hPa (Pour point)***
Method DIN ISO 3016***
Boiling point/range 380,3 °F (193,5 °C) @ 1 atm (101,3 kPa)
Method OECD 103***
Flash point 168,8 °F (76 °C) @ 1 atm (101,3 kPa)***
Method ISO 2719
Evaporation rate No data available
Flammability (solid, gas) Does not apply, the substance is a liquid
Lower explosion limit No data available
Upper explosion limit No data available

Vapour pressure

Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
2	0,2	0,002	20	68	
7,6	0,76	0,008	50	122	

Vapour density 5,0 (Air = 1) @ 20 °C (68 °F)

Relative density

Values	@ °C	@ °F	Method
0,8264	20	68	DIN 51757

Solubility 0,4 g/l @ 20 °C (68 °F), in water, OECD 105

log Pow 3,7 (measured) OECD 117

Autoignition temperature 725 °F (385 °C)

Method EU A.15

Decomposition temperature No data available

Viscosity 14,19 mPa*s @ 68 °F (20 °C)

Method dynamic, ASTM D445***

9.2. Other information

Molecular weight 144,26

Molecular formula C₉H₂₀O

log Koc 3,11 calculated***

Oxidizing properties Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties

Refractive Index 1,432 @ 68 °F (20 °C)***

Explosive properties Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties

Surface tension 38,0 mN/m (0,37 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

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text book on organic chemistry.

10.2. Chemical stability

Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

Vapour/air-mixtures are explosive at intense warming. 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

strong acids, strong oxidizing agents.

10.6. Hazardous decomposition products

No decomposition if used 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-Trimethylhexan-1-ol, CAS: 3452-97-9

Main symptoms

cough, nausea, gastrointestinal discomfort, vomiting.

Target Organ Systemic Toxicant - Single exposure

Due to lack of data, a classification is not possible for:

STOT SE

Target Organ Systemic Toxicant - Repeated exposure

Liver effects

Kidney disorders

The available data lead to the classification given in section 2

Acute toxicity

3,5,5-Trimethylhexan-1-ol (3452-97-9)

Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	> 2000 mg/kg	rat, male/female	OECD 401
Oral	LD50	2300 mg/kg	rat, male/female	OECD 401
Dermal	LD50	2307 mg/kg	rabbit	OECD 402

3,5,5-Trimethylhexan-1-ol, CAS: 3452-97-9

Assessment

Based on available data, the classification criteria are not met for:

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Acute oral toxicity

Acute dermal toxicity

Acute inhalation toxicity

An LC50/inhalation/4h/rat could not be determined because no mortality of rats was observed at the maximum achievable concentration

Irritation and corrosion				
3,5,5-Trimethylhexan-1-ol (3452-97-9)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	Moderate skin irritation	OECD 404	4h
Eyes	rabbit	Mild eye irritation***	OECD 405	

3,5,5-Trimethylhexan-1-ol, CAS: 3452-97-9

Assessment

The available data lead to the classification given in section 2

For respiratory irritation, no data are available

Sensitization				
3,5,5-Trimethylhexan-1-ol (3452-97-9)				
Target Organ Effects	Species	Evaluation	Method	
Skin	Human experience	not sensitizing	OECD 406	

3,5,5-Trimethylhexan-1-ol, CAS: 3452-97-9

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-Trimethylhexan-1-ol (3452-97-9)				
Type	Dose	Species	Method	
Subacute toxicity***	NOAEL: 12 mg/kg/d	rat, male/female	OECD 422	Oral
Subacute toxicity***	LOAEL: 60 mg/kg/d	rat, male/female	OECD 422	Oral

3,5,5-Trimethylhexan-1-ol, CAS: 3452-97-9

Assessment

The available data lead to the classification given in section 2

Carcinogenicity, Mutagenicity, Reproductive toxicity					
3,5,5-Trimethylhexan-1-ol (3452-97-9)					
Type	Dose	Species	Evaluation	Method	
Reproductive toxicity	NOAEL 300 mg/kg/d	rat, parental, male		OECD 422, Oral	
Reproductive toxicity	NOAEL 60 mg/kg/d	rat, parental, female		OECD 422, Oral	
Reproductive toxicity	NOAEL 12 mg/kg/d	rat, 1. Generation, male/female		OECD 422, Oral	

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Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	In vitro study
Mutagenicity		Escherichia coli	negative	OECD 472	In vitro study
Mutagenicity		CHL (Chinese hamster lung cells)***	negative	OECD 473 (Chromosomal Aberration)	In vitro study
Developmental Toxicity	NOAEL 12 mg/kg/d	rat		OECD 422	Maternal toxicity, Embryotoxicity
Developmental Toxicity	NOAEL 12 mg/kg/d	rat		OECD 422	Fetal toxicity
Developmental Toxicity	NOAEL 300 mg/kg/d	rat		OECD 422	Teratogenicity

3,5,5-Trimethylhexan-1-ol, CAS: 3452-97-9

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
No developmental effects in the absence of maternal toxicity

3,5,5-Trimethylhexan-1-ol, CAS: 3452-97-9

Aspiration toxicity

Due to the viscosity, this product does not present an aspiration hazard

Other adverse effects

Components of the product may be absorbed into the body by inhalation, ingestion and through the skin.

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-Trimethylhexan-1-ol (3452-97-9)			
Species	Exposure time	Dose	Method
Oryzias latipes (Medaka)	96h	LC50: 27,7 mg/l	OECD 203
Daphnia magna (Water flea)	48h	EC50: 6,77 mg/l***	OECD 202
Scenedesmus capricornutum (fresh water algae)	72h	EC50: > 33,3 mg/l (Biomass)	OECD 201
Scenedesmus capricornutum (fresh water algae)	72h	NOEC: 4,7 mg/l (Biomass)	OECD 201

Long term toxicity

3,5,5-Trimethylhexan-1-ol (3452-97-9)

Type	Species	Dose	Method	
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Mortality	Daphnia magna (Water flea)	LC50: > 3,87 mg/l	OECD 202	21 d
Reproductive toxicity	Daphnia magna (Water flea)	EC50: 2,09 mg/l	OECD 202	21 d
Aquatic toxicity***	Oryzias latipes (Medaka)	LC50: > 17 mg/l	OECD 204	14 d***
Aquatic toxicity***	Oryzias latipes (Medaka)	NOEC: 1,28 mg/l	OECD 204	14 d***
Aquatic toxicity***	Scenedesmus capricornutum (fresh water algae)***	NOEC: 10,3 mg/l Growth rate***	OECD 201***	3 d***

Terrestrial toxicity

3,5,5-Trimethylhexan-1-ol (3452-97-9)

Species	Exposure time	Dose	Type	Method
Xenopus laevis (African clawed frog)***	48 h***	LC50: 13,5 mg/l***	Mortality***	

12.2. Persistence and degradability

3,5,5-Trimethylhexan-1-ol, CAS: 3452-97-9

Biodegradation

3,67 % (28 d), BOD, activated sludge, Not readily biodegradable, OECD 301 C.***

Abiotic Degradation

3,5,5-Trimethylhexan-1-ol (3452-97-9)

Type	Result	Method
Hydrolysis***	not expected***	
Photolysis***	Half-life (DT50): 36 h***	calculated***

12.3. Bioaccumulative potential

3,5,5-Trimethylhexan-1-ol (3452-97-9)

Type	Result	Method
BCF	3,9 - 8,1 @ 100 µg/l	OECD 305 C
log Pow	3,7 @ 25 °C (77 °F)***	measured, OECD 117

12.4. Mobility in soil

3,5,5-Trimethylhexan-1-ol (3452-97-9)

Type	Result	Method
Surface tension	38,0 mN/m (0,37 g/l @ 20°C (68°F))	OECD 115
Adsorption/Desorption***	log Koc: 3,11***	calculated***
Distribution to environmental compartments***	Air: 9,9 % Soil: 83,1 % Water: 6,2 % Sediment: 0,8 %***	Calculation according Mackay, Level III***

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12.5. Results of PBT and vPvB assessment

3,5,5-Trimethylhexan-1-ol, CAS: 3452-97-9

PBT and vPvB assessment

Not required

12.6. Other adverse effects

3,5,5-Trimethylhexan-1-ol, CAS: 3452-97-9

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)

14.1. UN number	NA 1993
14.2. UN proper shipping name	Combustible liquid, n.o.s. (Isononanol)
14.3. Transport hazard class(es)	3
14.4. Packing group	III
14.5. Environmental hazards	no
14.6. Special precautions for user	
Emergency Response Guide	128
Remarks	Only regulated if over 119 gallons

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Not restricted

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IMDG

Not restricted

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

Product name	Nonyl alcohol
Ship type	2
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

State Regulations

3,5,5-Trimethylhexan-1-ol, CAS: 3452-97-9

MA RTK List
NY RTK List
PA RTK List

International Inventories

3,5,5-Trimethylhexan-1-ol, CAS: 3452-97-9

AICS (AU)
DSL (CA)
IECSC (CN)
EC-No. 2223767 (EU)
ENCS (2)-217 (JP)
ISHL (2)-217 (JP)
KECI KE-34566 (KR)
PICCS (PH)
TSCA (US)
NZIoC (NZ)***
TCSI (TW)

SECTION 16: Other information

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Hazard Rating Systems

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NFPA (National Fire Protection Association)

Health Hazard	2
Fire Hazard	2
Reactivity	0

HMIS (Hazardous Material Information System)

Health Hazard	2
Flammability	2
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

Observe national and local legal requirements. Changes against the previous version are marked by ***. The use of a comma in section 3 and section 7 to 12 is the same as a period.

Disclaimer

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End of Safety Data Sheet