SECTION 1: Identification of the substance / mixture and of the company / undertaking

1.1. Product identifier

Identification of the substance/preparation **Isononanol**

Chemical Name	3,5,5-Trimethylhexan-1-ol
CAS-No	3452-97-9
EC No.	222-376-7
Registration number (REACh)	01-2119937262-41

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

Identified uses	Transported isolated intermediate (1907/2006)
Uses advised against	None

1.3. Details of the supplier of the safety data sheet

Company/Undertaking Identification	**OQ Chemicals GmbH** Rheinpromenade 4A D-40789 Monheim Germany
Product Information	Product Stewardship FAX: +49 (0)208 693 2053 email: sc.psq@oq.com

1.4. Emergency telephone number

Emergency telephone number	+65 3158 1074 (Singapore) available 24/7
Local emergency telephone number	+886 2 8793 3212 available 24/7

2. Hazards identification

Basis for Classification This substance is classified based on GHS (United Nations version 2017)

Classification

Flammable liquid	Category 4
Acute oral toxicity	Category 5
Acute dermal toxicity	Category 5
Skin corrosion/irritation	Category 2
Serious eye damage/eye irritation	Category 2A
Target Organ Systemic Toxicant - Repeated exposure	Category 2
Environmental hazard	Acute aquatic toxicity 2

Hazard pictograms

Signal word **Warning**

Hazard statements

H227: Combustible liquid
H303: May be harmful if swallowed
H313: May be harmful in contact with skin
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

P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P260: Do not breathe gas/mist/vapours.
P280: Wear protective gloves/protective clothing/eye protection/face protection.
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.
P312: Call a POISON CENTRE/doctor if you feel unwell.
P403 + P235: Store in a well ventilated place. Keep cool.

Other Hazards

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

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 plenty of water for at least 15 minutes. When symptoms persist or in all cases of doubt

seek medical advice.

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
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

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.

Temperature class
T2

7.3. Specific end use(s)

Transported isolated intermediate (1907/2006)

SECTION 8: Exposure controls / personal protection

Exposure limits Japan

No exposure limits established.

Occupational Exposure Controls

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.

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 (dust). Equipment should conform to NIOSH, EN or other applicable national standards.

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
Colour	colourless
Odour	alcoholic
Odour threshold	No data available
pH	No data available
Melting point/range	-80 °C @ 1013 hPa (Pour point)
Boiling point/range	193,5 °C @ 1013 hPa
Flash point	76 °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	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, in water, OECD 105
log Pow	3,7 (measured), OECD 117
Autoignition temperature	385 °C
Method	EU A.15
Decomposition temperature	No data available
Viscosity	14,19 mPa*s @ 20 °C
Method	dynamic, ASTM D445
Oxidizing properties	Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties
Explosive properties	Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties

9.2. Other information

Molecular weight	144,26
Molecular formula	C9 H20 O
log Koc	3,11 calculated
Refractive index	1,432 @ 20 °C
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 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

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:
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	
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	In vitro study
Mutagenicity		Escherichia coli	negative	OECD 472	In vitro study
Mutagenicity		CHL (Chinese	negative	OECD 473	In vitro study

		hamster lung cells)		(Chromosomal Aberration)	
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
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
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	
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

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

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	Nonyl alcohol
Ship type	2
Pollution category	Y

SECTION 15: Regulatory information

GHS

Classification

This substance is classified based on GHS (United Nations version 2017).
(See chapter 2)

National regulatory information Japan

NITE GHS

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

ID-No.	ID 448
Classification	Flammable liquid: category 4 Acute oral toxicity: category 4 Acute dermal toxicity: category 5 Skin corrosion/irritation: category 2 Serious eye damage/eye irritation: category 2B Toxic to reproduction: category 2 Target Organ Systemic Toxicant - Repeated exposure: category 2 Acute hazard to the aquatic environment: category 2 Chronic hazard to the aquatic environment: category 2
Target organs - repeated exposure	Hazard category 2: Kidney Liver
Symbols	Exclamation mark Health Hazard Environment
Signal word	Warning
Hazard statements	H227, H302, H313, H315, H320, H361, H373, H401, H411
Prevention	P210, P280b, P264, P270, P201, P202, P281, P260, P273
Response	P370+P378, P301+P312, P330, P302+P352, P321, P332+P313, P362, P305+P351+P338, P337+P313, P308+P313, P314, P391
Storage	P403+P235, P405
Disposal	P501

JAISH-GHS Classification list
not listed

Poisonous and Deleterious Substances Control Law
not listed

Poisonous and Deleterious Substances Cabinet Order
not listed

ISHL Enforcement Order, Article 17, Table 3-1
not listed

ISHL Enforcement Order 35, Article 18-2
not listed

ISHL Enforcement Order, Table 3
not listed

ISHL Enforcement Order, Table 6-2 Organic solvents
not listed

ISHL Enforcement Order, Table 1-1 to 1-5
not listed

ISHL Corrosive liquids, Art. 326
not listed

ISHL Designated carcinogens
not listed

ISHL Mutagens
not listed

ISHL Prohibited Substances
not listed

ISHL Enforcement Order 349, Article 18
not listed

ISHL Ordinance No. 39, Specified chemical substances
not listed
Fire Service law:
not listed
Marine Pollutant prevention law
not listed
PRTR Substances (Cabinet Order 138)

PRTR Substances (Cabinet Order 356)

Component	Class	Specified Class	Item No.	Annual threshold reporting quantity	Threshold limits
3,5,5-Trimethylhexan-1-ol 3452-97-9 (> 97,5)	1		295	1 TONS	1 %WT

PDSCL Enforcement Order Article 32-3
not listed
Water Pollutants, Hazardous to human health, Standard No. 35, Table 1
not listed
Water Pollutants, Harmful to the environment, Standard No. 35, Table 2
not listed

For details and further information please refer to the original regulation

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

Abbreviations
A table of terms and abbreviations can be found under the following link:
http://echa.europa.eu/documents/10162/13632/information_requirements_r20_en.pdf

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 ***.

Disclaimer
For industrial use only. The information contained herein is accurate to the best of our knowledge. We do not suggest or guarantee that any hazards listed herein are the only ones which exist. OQ makes no warranty of any kind, express or implied, concerning the safe use of this material in your process or in combination with other substances. User has the sole responsibility to determine the suitability of the materials for any use and the manner of use contemplated. User must meet all applicable safety and health standards

End of Safety Data Sheet