

Safety data sheet

acc. to Safe Work Australia - Code of Practice



Isooctane $\geq 99,5$ %, for synthesis

article number: **9860**
Version: **GHS 4.0 en**
Replaces version of: 2022-05-06
Version: (GHS 3)

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Revision: 2024-03-03

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

1.1 Product identifier

Identification of the substance	Isooctane $\geq 99,5$ %, for synthesis
Article number	9860
CAS number	540-84-1
Alternative name(s)	2,2,4-Trimethylpentane

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household). Food, drink and animal feeding-stuffs.

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

Telephone: +49 (0) 721 - 56 06 0
Telefax: +49 (0) 721 - 56 06 149
e-mail: sicherheit@carlroth.de
Website: www.carlroth.de

Competent person responsible for the safety data sheet: Department Health, Safety and Environment

e-mail (competent person): sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 Westmead, NSW	131126	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
2.6	Flammable liquid	2	Flam. Liq. 2	H225
3.2	Skin corrosion/irritation	2	Skin Irrit. 2	H315
3.8D	Specific target organ toxicity - single exposure (narcotic effects, drowsiness)	3	STOT SE 3	H336

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Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.10	Aspiration hazard	1	Asp. Tox. 1	H304

For full text of abbreviations: see SECTION 16

The most important adverse physicochemical, human health and environmental effects

The product is combustible and can be ignited by potential ignition sources.

2.2 Label elements

Labelling

Signal word

Danger

Pictograms

GHS02, GHS07,
GHS08



Hazard statements

H225 Highly flammable liquid and vapour
H304 May be fatal if swallowed and enters airways
H315 Causes skin irritation
H336 May cause drowsiness or dizziness

Precautionary statements

Precautionary statements - prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking

Precautionary statements - response

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
P302+P352 IF ON SKIN: Wash with plenty of soap and water
P331 Do NOT induce vomiting
P370+P378 In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction

Precautionary statements - storage

P403+P233 Store in a well-ventilated place. Keep container tightly closed
P403+P235 Store in a well-ventilated place. Keep cool

2.3 Other hazards

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

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SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Isooctane
Molecular formula	C_8H_{18}
Molar mass	114.2 g/mol
CAS No	540-84-1

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In case of skin irritation, consult a physician.

Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

Following ingestion

Rinse mouth. Do not induce vomiting. Observe aspiration hazard if vomiting occurs. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

Following inhalation: Drowsiness, Dizziness, Narcosis,
Following skin contact: Irritation,
After eye contact: Irritant effects,
Following ingestion: Aspiration hazard

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!
water spray, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

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Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours may form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO₂)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it. If substance has entered a water course or sewer, inform the responsible authority.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains.

Advice on how to clean up a spill

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation.

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Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge. Due to danger of explosion, prevent leakage

of vapours into cellars, flues and ditches.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs. When using do not smoke.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Ground/bond container and receiving equipment.

Ventilation requirements

Use local and general ventilation.

Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °C

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	2,035 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	773 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

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8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



• hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

• type of material

NBR (Nitrile rubber)

• material thickness

>0,3 mm

• breakthrough times of the glove material

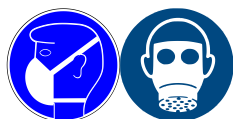
>480 minutes (permeation: level 6)

• other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Flame-retardant protective clothing.

Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C, colour code: Brown).

Environmental exposure controls

Keep away from drains, surface and ground water.

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SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	colourless
Odour	like: Gasoline
Melting point/freezing point	-107 °C
Boiling point or initial boiling point and boiling range	99.2 °C at 1,013 hPa
Flammability	flammable liquid in accordance with GHS criteria
Lower and upper explosion limit	45 g/m ³ (LEL) - 290 g/m ³ (UEL) / 1 vol% (LEL) - 6 vol% (UEL)
Flash point	-12 °C (ECHA)
Auto-ignition temperature	418 °C (ECHA) (auto-ignition temperature (liquids and gases))
Decomposition temperature	not relevant
pH (value)	(20 °C) (neutral)
Kinematic viscosity	not determined
Dynamic viscosity	0.5 mPa s at 20 °C
<u>Solubility(ies)</u>	
Water solubility	(poorly soluble (1 till < 10 mg/l))
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	4.08 (ECHA)
Soil organic carbon/water (log KOC)	2.38 (ECHA)
Vapour pressure	28 hPa at 20 °C
<u>Density and/or relative density</u>	
Density	0.69 g/cm ³ at 15 °C
Relative vapour density	3.9 (air = 1)
Particle characteristics	not relevant (liquid)
<u>Other safety parameters</u>	
Oxidising properties	none
Information with regard to physical hazard classes:	There is no additional information.

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Other safety characteristics:

Gas group (explosion group)	IIA Maximum Experimental Safe Gap value; MESG > 0,9 mm
Maximum explosion pressure	9 bar
Surface tension	18.77 mN/m (20 °C) (ECHA)
Refractive index	1.392

SECTION 10: Stability and reactivity

10.1 Reactivity

It's a reactive substance. Risk of ignition. Vapours may form explosive mixtures with air.

If heated

Risk of ignition.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser

10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. UV-radiation/sunlight.

10.5 Incompatible materials

different plastics

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Shall not be classified as acutely toxic.

GHS of the United Nations, annex 4. May be harmful in contact with skin or if inhaled.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	>5,000 mg/kg	rat		ECHA
inhalation: vapour	LC50	>33.52 mg/l/4h	rat		ECHA
dermal	LD50	>2,000 mg/kg	rabbit		ECHA

Skin corrosion/irritation

Causes skin irritation.

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Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

May be fatal if swallowed and enters airways.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

vomiting, aspiration hazard

• If in eyes

causes slight to moderate irritation

• If inhaled

drowsiness, dizziness, fatigue, narcosis

• If on skin

causes skin irritation

• Other information

none

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

SECTION 12: Ecological information

12.1 Toxicity

Very toxic to aquatic life with long lasting effects.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LL50	18.4 mg/l	fish	ECHA	96 h
LC50	0.11 mg/l	fish	ECHA	96 h

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Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
EC50	0.4 mg/l	aquatic invertebrates	ECHA	48 h
EL50	2.4 mg/l	aquatic invertebrates	ECHA	48 h

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
EL50	1.6 mg/l	aquatic invertebrates	ECHA	21 d
EC50	0.23 mg/l	aquatic invertebrates	ECHA	21 d

12.2 Persistence and degradability

Theoretical Oxygen Demand: 3.501 mg/mg
Theoretical Carbon Dioxide: 3.082 mg/mg

Process of degradability		
Process	Degradation rate	Time
oxygen depletion	61.81 %	70 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	4.08 (ECHA)
BCF	231 (ECHA)

12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	2.38 (ECHA)
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12.5 Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.

12.7 Other adverse effects

Data are not available.

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SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

Only packagings which are approved (e.g. acc. to the Dangerous Goods Regulations) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

Relevant provisions relating to waste(Basel Convention)

Properties of waste which render it hazardous

H3 Flammable liquids
H11 Toxic (Delayed or chronic)

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

SECTION 14: Transport information

14.1 UN number

UN RTDG	UN 1262
IMDG-Code	UN 1262
ICAO-TI	UN 1262

14.2 UN proper shipping name

UN RTDG	OCTANES
IMDG-Code	OCTANES
ICAO-TI	Octanes

14.3 Transport hazard class(es)

UN RTDG	3
IMDG-Code	3
ICAO-TI	3

14.4 Packing group

UN RTDG	II
IMDG-Code	II
ICAO-TI	II

14.5 Environmental hazards

hazardous to the aquatic environment

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14.6 Special precautions for user

There is no additional information.

14.7 Transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

14.8 Information for each of the UN Model Regulations

Transport information National regulations Additional information (UN RTDG)

UN number	1262
Class	3
Environmental hazards	Yes Hazardous to the aquatic environment
Packing group	II
Danger label(s)	3 Fish and tree



Special provisions (SP)	- UN RTDG
Excepted quantities (EQ)	E2 UN RTDG
Limited quantities (LQ)	1 L UN RTDG
Emergency Action Code	3YE

International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name	OCTANES
Particulars in the shipper's declaration	UN1262, OCTANES, 3, II, -12°C c.c., MARINE POLLUTANT
Marine pollutant	yes (P) (hazardous to the aquatic environment)
Danger label(s)	3, "Fish and tree"



Special provisions (SP)	-
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
EmS	F-E, S-E
Stowage category	B

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International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Proper shipping name	Octanes
Particulars in the shipper's declaration	UN1262, Octanes, 3, II
Environmental hazards	yes (hazardous to the aquatic environment)
Danger label(s)	3



Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

There is no additional information.

National regulations(Australia)

Australian Inventory of Chemical Substances(AICS)

Substance is listed.

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

Legend

AIIC	Australian Inventory of Industrial Chemicals
CICR	Chemical Inventory and Control Regulation
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)

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Legend

ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.	yes
14.8		Emergency Action Code: 3YE	yes
15.1		Other information: Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.	yes
15.1		National inventories: change in the listing (table)	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
EL50	Effective Loading 50 %: the EL50 corresponds to the loading rate required to produce a response in 50% of the test organisms
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association

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Abbr.	Descriptions of used abbreviations
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
LEL	Lower explosion limit (LEL)
LL50	Lethal Loading 50 %: the LL50 corresponds to the loading rate causing 50 % lethality
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
UEL	Upper explosion limit (UEL)
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.