

safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Isooctane ≥99,5 %, for synthesis

article number: **9860**
Version: **GHS 1.0 en**

date of compilation: 13.01.2016

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

1.1 Product identifier

Identification of the substance	ISOOCTANE ≥ 99.5%, for synthesis
Article number	9860
Registration number (REACH)	01-2119457965-22-xxxx
Index No	601-009-00-8
EC number	208-759-1
CAS number	540-84-1

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

Identified uses: laboratory chemical

1.3 Details of the supplier of the safety data sheet

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

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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

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
2.6	flammable liquid	(Flam. Liq. 2)	H225
3.2	skin corrosion/irritation	(Skin Irrit. 2)	H315
3.8D	specific target organ toxicity - single exposure (narcotic effects, drowsiness)	(STOT SE 3)	H336
3.10	aspiration hazard	(Asp. Tox. 1)	H304
4.1A	hazardous to the aquatic environment - acute hazard	(Aquatic Acute 2)	H401
4.1C	hazardous to the aquatic environment - chronic hazard	(Aquatic Chronic 2)	H411

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Remarks

For full text of Hazard- and EU Hazard-statements: see SECTION 16.

The most important adverse physicochemical, human health and environmental effects

Narcotic effects.

2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 (CLP)

Signal word

Danger

Pictograms



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.
H411	Toxic to aquatic life with long lasting effects.

Precautionary statements

Precautionary statements - prevention

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
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Precautionary statements - response

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

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.

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)



H304	May be fatal if swallowed and enters airways.
H401	Toxic to aquatic life.
P331	Do NOT induce vomiting.

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2.3 Other hazards

There is no additional information.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	2,2,4-trimethylpentane
Index No	601-009-00-8
Registration number (REACH)	01-2119457965-22-xxxx
EC number	208-759-1
CAS number	540-84-1
Molecular formula	$C_8 H_{18}$
Molar mass	114,2 g/mol

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing. If breathing is irregular or stopped, immediately seek medical assistance and start first aid actions.

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. Call a physician immediately. Observe aspiration hazard if vomiting occurs.

4.2 Most important symptoms and effects, both acute and delayed

Aspiration hazard, Dizziness, Unconsciousness, Headache, Pulmonary oedema, Gastrointestinal complaints, Cough, Vertigo, Nausea, Pneumonia, Irritation, Vomiting

4.3 Indication of any immediate medical attention and special treatment needed

none

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SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings
foam, dry extinguishing powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours are heavier than air, spread along floors and form explosive mixtures with air.
Vapours can 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

Do not allow firefighting water to enter drains or water courses. 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

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. 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 it. Explosive properties.

6.3 Methods and material for containment and cleaning up

Advices on how to contain a spill

Covering of drains.

Advices on how to clean up a spill

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

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

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.

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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation. Avoid: Aerosol or mist formation.

• 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)

not relevant

Relevant DNELs/DMELs/PNECs and other threshold levels

• human health values

Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	773 mg/kg	human, dermal	worker (industry)	chronic - systemic effects
DNEL	2.035 mg/m ³	human, inhalatory	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.

• type of material

NBR (Nitrile rubber)

• material thickness

0,4 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).

Observe the wear time limits according GefStoffV in combination with the rules for using respiratory protection apparatus (BGR 190).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance

Physical state	liquid (fluid)
Colour	colourless
Odour	like: Gasoline
Odour threshold	No data available

Other physical and chemical parameters

pH (value)	This information is not available.
Melting point/freezing point	-107 °C
Initial boiling point and boiling range	99,2 °C at 100 kPa
Flash point	-12 °C (closed cup)
Evaporation rate	no data available
Flammability (solid, gas)	not relevant (fluid)

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Explosive limits

• lower explosion limit (LEL)	1 vol% (45 g/m ³)
• upper explosion limit (UEL)	6 vol% (290 g/m ³)
Explosion limits of dust clouds	not relevant
• upper explosion limit (UEL)	290 g/m ³
Vapour pressure	2,8 kPa at 20 °C
Density	0,69 g/cm ³ at 15 °C
Vapour density	3,9 air = 1
Bulk density	Not applicable
Relative density	Information on this property is not available.

Solubility(ies)

Water solubility 2,2 mg/l at 25 °C

Partition coefficient

n-octanol/water (log KOW)	4,09 (TOXNET)
Soil organic carbon/water (log KOC)	4,35
Auto-ignition temperature	418 °C - ECHA
Decomposition temperature	no data available
Viscosity	
• dynamic viscosity	0,5 mPa s at 20 °C
Explosive properties	none
Oxidising properties	none

9.2 Other information

Surface tension	18,77 mN/m (20 °C)
Refractive index	1,392

SECTION 10: Stability and reactivity

10.1 Reactivity

risk of ignition. Vapours can form explosive mixtures with air.

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

Exothermic reaction with: Strong oxidiser

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10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

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

Acute toxicity

Shall not be classified as acutely toxic.

Exposure route	Endpoint	Value	Species	Source
oral	LD50	$>5.000 \text{ mg/kg}$	rat	ECHA
inhalation: vapour	LC50	$>33,52 \text{ mg/l/4h}$	rat	ECHA
dermal	LD50	$>2.000 \text{ mg/kg}$	rabbit	ECHA

Skin corrosion/irritation

Causes skin irritation.

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.

Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor 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, varying degrees of pulmonary injury, nausea, aspiration hazard

- **If in eyes**

slightly irritant

- **If inhaled**

vertigo, headache

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• If on skin

causes skin irritation, repeated exposure may cause skin dryness or cracking

Other information

Dyspnoea, Narcosis

SECTION 12: Ecological information

12.1 Toxicity

Toxic to aquatic life. Toxic to aquatic life with long lasting effects.

Aquatic toxicity (acute)

Toxic to aquatic organisms.

Endpoint	Value	Species	Source	Exposure time
EL50	2,943 mg/l	algae	ECHA	72 hours

Aquatic toxicity (chronic)

May cause long-term adverse effects in the aquatic environment.

12.2 Process of degradability

Theoretical Oxygen Demand: 3,501 mg/mg

Theoretical Carbon Dioxide: 3,082 mg/mg

12.3 Bioaccumulative potential

The substance fulfils the very bioaccumulative criterion.

n-octanol/water (log KOW) 4,09

12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient 4,35

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Other adverse effects

Hazardous to water.

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. Avoid release to the environment. Refer to special instructions/safety data sheets.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

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13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

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.

SECTION 14: Transport information

14.1	UN number	1262
14.2	UN proper shipping name	OCTANES
	Hazardous ingredients	ISOCTANE $\geq 99.5\%$, for synthesis
14.3	Transport hazard class(es)	
	Class	3 (flammable liquids)
14.4	Packing group	II (substance presenting medium danger)
14.5	Environmental hazards	hazardous to the aquatic environment
14.6	Special precautions for user	
	Provisions for dangerous goods (ADR) should be complied within the premises.	
14.7	Transport in bulk according to Annex II of MARPOL and the IBC Code	
	The cargo is not intended to be carried in bulk.	
14.8	Information for each of the UN Model Regulations	
	• Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)	
	UN number	1262
	Proper shipping name	OCTANES
	Particulars in the transport document	UN1262, OCTANES, 3, II, (D/E), environmentally hazardous
	Class	3
	Classification code	F1
	Packing group	II
	Danger label(s)	3 + "fish and tree"
	 	
	Environmental hazards	yes (hazardous to the aquatic environment)
	Excepted quantities (EQ)	E2
	Limited quantities (LQ)	1 L
	Transport category (TC)	2
	Tunnel restriction code (TRC)	D/E
	Hazard identification No	33

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• International Maritime Dangerous Goods Code (IMDG)

UN number	1262
Proper shipping name	OCTANES
Particulars in the shipper's declaration	UN1262, OCTANES, (2,2,4-trimethylpentane), 3, II, -12°C c.c., MARINE POLLUTANT
Class	3
Marine pollutant	yes (hazardous to the aquatic environment)
Packing group	II
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

SECTION 15: Regulatory information

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

Relevant provisions of the European Union (EU)

- **Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)**
Not listed.
- **Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)**
Not listed.
- **Regulation 850/2004/EC on persistent organic pollutants (POP)**
Not listed.
- **Restrictions according to REACH, Annex XVII**
not listed
- **List of substances subject to authorisation (REACH, Annex XIV)**
not listed
- **Seveso Directive**

2012/18/EU (Seveso III)				
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements		Notes
P5c	flammable liquids (cat. 2, 3)	5.000	50.000	51)
E1	environmental hazards (hazardous to the aquatic environment, cat. 1)	100	200	56)

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Notation

- 51) Flammable liquids, categories 2 or 3 not covered by P5a and P5b
- 56) Hazardous to the Aquatic Environment in category Acute 1 or Chronic 1

• Limitation of emissions of volatile organic compounds due to the use of organic solvents in certain paints and varnishes and vehicle refinishing products (2004/42/EC, Deco-Paint Directive)

VOC content 100 %

• Directive on industrial emissions (VOCs, 2010/75/EU)

VOC content 100 %

Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II

not listed

Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)

not listed

National inventories

Substance is listed in the following national inventories:

- EINECS/ELINCS/NLP (Europe)
- REACH (Europe)

15.2 Chemical Safety Assessment

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

SECTION 16: Other information

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
EINECS	European Inventory of Existing Commercial Chemical Substances
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
IMDG	International Maritime Dangerous Goods Code
index No	the Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008

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Abbr.	Descriptions of used abbreviations
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
VOC	Volatile Organic Compounds
vPvB	very Persistent and very Bioaccumulative

Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)

List of relevant phrases (code and full text as stated in chapter 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
H401	toxic to aquatic life
H411	toxic to aquatic life with long lasting effects

Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.