

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: **6889**  
Version: **4.0 en**  
Replaces version of: 2022-05-06  
Version: (3)

date of compilation: 2016-01-13  
Revision: 2024-03-03

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

### 1.1 Product identifier

|                                 |  |
|---------------------------------|--|
| Identification of the substance | <b>Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS</b> |
| Article number                  | 6889   |
| Registration number (REACH)     | 01-2119457965-22-xxxx                          |
| Index number in CLP Annex VI    | 601-009-00-8                                   |
| EC number                       | 208-759-1                                      |
| 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<br>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](mailto:sicherheit@carlroth.de)  
**Website:** [www.carlroth.de](http://www.carlroth.de)

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

**e-mail (competent person):** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

### 1.4 Emergency telephone number

| Name   | Street        | Postal code/city | Telephone       | Website   |
|--|---------------|------------------|-----------------|---|
| National Poisons Information Centre<br>Beaumont Hospital | Beaumont Road | Dublin 9         | +353 1 809 2166 | <a href="https://www.poisons.ie/">https://www.poisons.ie/</a> |

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

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

| 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             |
| 3.10    | Aspiration hazard   | 1         | Asp. Tox. 1               | H304             |
| 4.1A    | Hazardous to the aquatic environment - acute hazard                             | 1         | Aquatic Acute 1           | H400             |
| 4.1C    | Hazardous to the aquatic environment - chronic hazard                           | 1         | Aquatic Chronic 1         | H410             |

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. Spillage and fire water can cause pollution of watercourses.

### 2.2 Label elements

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

##### Signal word

**Danger**

##### Pictograms

GHS02, GHS07,  
GHS08, GHS09



##### 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  
H410 Very toxic to aquatic life with long lasting effects

##### Precautionary statements

###### Precautionary statements - prevention

P210 Keep away from heat, sparks, open flames, hot surfaces. No smoking  
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection

###### Precautionary statements - response

P301+P330+P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting  
P302+P352 IF ON SKIN: Wash with plenty of soap and water  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P312 Call a POISON CENTRE/doctor if you feel unwell

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

### Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)



H304  
H336

May be fatal if swallowed and enters airways.  
May cause drowsiness or dizziness.

P304+P340  
P312

IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
Call a POISON CENTRE/doctor if you feel unwell.

## 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 ≥ 0,1%.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                   |                                |
|-------------------|--------------------------------|
| Name of substance | Isooctane                      |
| Molecular formula | C <sub>8</sub> H <sub>18</sub> |
| Molar mass        | 114,2 g/mol                    |
| REACH Reg. No     | 01-2119457965-22-xxxx          |
| CAS No            | 540-84-1                       |
| EC No             | 208-759-1                      |
| Index No          | 601-009-00-8                   |

## 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.

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

### 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 (CO<sub>2</sub>)

#### 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 (CO<sub>2</sub>)

### 5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. 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

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.

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

### 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.

#### 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.

#### Measures to protect the environment

Avoid release to the environment.

#### 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.

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

## 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 <sup>3</sup> | human, inhalatory                  | worker (industry) | chronic - systemic effects |
| DNEL                                      | 773 mg/kg bw/day        | human, dermal                      | worker (industry) | chronic - systemic effects |

### 8.2 Exposure controls

#### Individual protection measures (personal protective equipment)

##### Eye/face protection



Use safety goggles 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)

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

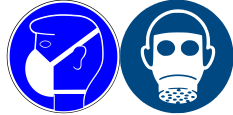
article number: 6889

### • 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.

## 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 <sup>3</sup> (LEL) - 290 g/m <sup>3</sup> (UEL) /<br>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   |

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

### Density and/or relative density

|                         |                                 |
|-------------------------|---------------------------------|
| Density                 | 0,69 g/cm <sup>3</sup> at 15 °C |
| Relative vapour density | 3,9 (air = 1)                   |

Particle characteristics not relevant (liquid)

### Other safety parameters

Oxidising properties none

## 9.2 Other information

Information with regard to physical hazard classes: There is no additional information.

Other safety characteristics:

|                                      |   |
|--------------------------------------|---|
| Gas group (explosion group)          | IIA<br>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   |
| Temperature class (EU, acc. to ATEX) | T2<br>Maximum permissible surface temperature on the equipment: 300°C |

## 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.



# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

## SECTION 11: Toxicological information

### 11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Classification according to GHS (1272/2008/EC, CLP)

##### Acute toxicity

Shall not be classified as acutely toxic.

| 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.

##### 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

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

### • Other information

none

### 11.2 Endocrine disrupting properties

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

### 11.3 Information on other hazards

There is no additional information.

## 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          |
| 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)  |

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

### 12.4 Mobility in soil

|  |             |
|--|-------------|
| The Organic Carbon normalised adsorption coefficient | 2,38 (ECHA) |
|--|-------------|

### 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.

## 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. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

### 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.

#### Properties of waste which render it hazardous

- HP 3** flammable
- HP 4** irritant - skin irritation and eye damage
- HP 5** specific target organ toxicity (STOT)/aspiration toxicity
- HP 14** ecotoxic

### 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 or ID number

|           |         |
|-----------|---------|
| ADRRID    | UN 1262 |
| IMDG-Code | UN 1262 |
| ICAO-TI   | UN 1262 |

### 14.2 UN proper shipping name





# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: **6889**

|   |  |
|---|--|
| ADRRID  | OCTANES  |
| IMDG-Code   | OCTANES  |
| ICAO-TI   | Octanes  |
| <b>14.3 Transport hazard class(es)</b>  |  |
| ADRRID  | 3  |
| IMDG-Code   | 3  |
| ICAO-TI   | 3  |
| <b>14.4 Packing group</b>   |  |
| ADRRID  | II   |
| IMDG-Code   | II   |
| ICAO-TI   | II   |
| <b>14.5 Environmental hazards</b>   | hazardous to the aquatic environment                     |
| <b>14.6 Special precautions for user</b>  |  |
| Provisions for dangerous goods (ADR) should be complied within the premises.  |  |
| <b>14.7 Maritime transport in bulk according to IMO instruments</b>   |  |
| The cargo is not intended to be carried in bulk.  |  |
| <b>14.8 Information for each of the UN Model Regulations</b>  |  |
| <b>Agreement concerning the International Carriage of Dangerous Goods by Road (ADR)Additional information</b>   |  |
| Proper shipping name  | OCTANES  |
| Particulars in the transport document   | UN1262, OCTANES, 3, II, (D/E), environmentally hazardous |
| Classification code   | F1   |
| 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   |
| <b>Regulations concerning the International Carriage of Dangerous Goods by Rail (RID)Additional information</b>   |  |
| Classification code   | F1   |
| Danger label(s)   | 3, "Fish and tree"                                       |
|   |  |



# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

|   |  |
|---|--|
| <b>Environmental hazards</b>  | Yes<br>Hazardous to water                            |
| <b>Excepted quantities (EQ)</b>   | E2   |
| <b>Limited quantities (LQ)</b>  | 1 L  |
| <b>Transport category (TC)</b>  | 2  |
| <b>Hazard identification No</b>   | 33   |
| <b>International Maritime Dangerous Goods Code (IMDG) - Additional information</b>        |  |
| 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  |
| <b>International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information</b> |  |
| 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

#### Relevant provisions of the European Union (EU)

#### Restrictions according to REACH, Annex XVII

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

| Dangerous substances with restrictions (REACH, Annex XVII) |  |        |             |    |
|--|--|--------|-------------|----|
| Name of substance  | Name acc. to inventory   | CAS No | Restriction | No |
| Isooctane  | this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC |        | R3          | 3  |
| Isooctane  | flammable / pyrophoric   |        | R40         | 40 |
| Isooctane  | substances in tattoo inks and permanent make-up  |        | R75         | 75 |

### Legend

- R3
1. Shall not be used in:
    - ornamental articles intended to produce light or colour effects by means of different phases, for example in ornamental lamps and ashtrays,
    - tricks and jokes,
    - games for one or more participants, or any article intended to be used as such, even with ornamental aspects,
  2. Articles not complying with paragraph 1 shall not be placed on the market.
  3. Shall not be placed on the market if they contain a colouring agent, unless required for fiscal reasons, or perfume, or both, if they:
    - can be used as fuel in decorative oil lamps for supply to the general public, and
    - present an aspiration hazard and are labelled with H304.
  4. Decorative oil lamps for supply to the general public shall not be placed on the market unless they conform to the European Standard on Decorative oil lamps (EN 14059) adopted by the European Committee for Standardisation (CEN).
  5. Without prejudice to the implementation of other Union provisions relating to the classification, labelling and packaging of substances and mixtures, suppliers shall ensure, before the placing on the market, that the following requirements are met:
    - (a) lamp oils, labelled with H304, intended for supply to the general public are visibly, legibly and indelibly marked as follows: "Keep lamps filled with this liquid out of the reach of children"; and, by 1 December 2010, "Just a sip of lamp oil – or even sucking the wick of lamps – may lead to life-threatening lung damage";
    - (b) grill lighter fluids, labelled with H304, intended for supply to the general public are legibly and indelibly marked by 1 December 2010 as follows: "Just a sip of grill lighter fluid may lead to life threatening lung damage";
    - (c) lamps oils and grill lighters, labelled with H304, intended for supply to the general public are packaged in black opaque containers not exceeding 1 litre by 1 December 2010.;
- R40
1. Shall not be used, as substance or as mixtures in aerosol dispensers where these aerosol dispensers are intended for supply to the general public for entertainment and decorative purposes such as the following:
    - metallic glitter intended mainly for decoration,
    - artificial snow and frost,
    - 'whoopie' cushions,
    - silly string aerosols,
    - imitation excrement,
    - horns for parties,
    - decorative flakes and foams,
    - artificial cobwebs,
    - stink bombs.
  2. Without prejudice to the application of other Community provisions on the classification, packaging and labelling of substances, suppliers shall ensure before the placing on the market that the packaging of aerosol dispensers referred to above is marked visibly, legibly and indelibly with:  
'For professional users only'.
  3. By way of derogation, paragraphs 1 and 2 shall not apply to the aerosol dispensers referred to Article 8 (1a) of Council Directive 75/324/EEC (2).
  4. The aerosol dispensers referred to in paragraphs 1 and 2 shall not be placed on the market unless they conform to the requirements indicated.

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

### Legend

- R75
1. Shall not be placed on the market in mixtures for use for tattooing purposes, and mixtures containing any such substances shall not be used for tattooing purposes, after 4 January 2022 if the substance or substances in question is or are present in the following circumstances:
    - (a) in the case of a substance classified in Part 3 of Annex VI to Regulation (EC) No 1272/2008 as carcinogen category 1A, 1B or 2, or germ cell mutagen category 1A, 1B or 2, the substance is present in the mixture in a concentration equal to or greater than 0,00005 % by weight;
    - (b) in the case of a substance classified in Part 3 of Annex VI to Regulation (EC) No 1272/2008 as reproductive toxicant category 1A, 1B or 2, the substance is present in the mixture in a concentration equal to or greater than 0,001 % by weight;
    - (c) in the case of a substance classified in Part 3 of Annex VI to Regulation (EC) No 1272/2008 as skin sensitiser category 1, 1A or 1B, the substance is present in the mixture in a concentration equal to or greater than 0,001 % by weight;
    - (d) in the case of a substance classified in Part 3 of Annex VI to Regulation (EC) No 1272/2008 as skin corrosive category 1, 1A, 1B or 1C or skin irritant category 2, or as serious eye damage category 1 or eye irritant category 2, the substance is present in the mixture in a concentration equal to or greater than:
      - (i) 0,1 % by weight, if the substance is used solely as a pH regulator;
      - (ii) 0,01 % by weight, in all other cases;
    - (e) in the case of a substance listed in Annex II to Regulation (EC) No 1223/2009 (\*1), the substance is present in the mixture in a concentration equal to or greater than 0,00005 % by weight;
    - (f) in the case of a substance for which a condition of one or more of the following kinds is specified in column g (Product type, Body parts) of the table in Annex IV to Regulation (EC) No 1223/2009, the substance is present in the mixture in a concentration equal to or greater than 0,00005 % by weight:
      - (i) "Rinse-off products";
      - (ii) "Not to be used in products applied on mucous membranes";
      - (iii) "Not to be used in eye products";
    - (g) in the case of a substance for which a condition is specified in column h (Maximum concentration in ready for use preparation) or column i (Other) of the table in Annex IV to Regulation (EC) No 1223/2009, the substance is present in the mixture in a concentration, or in some other way, that does not accord with the condition specified in that column;
    - (h) in the case of a substance listed in Appendix 13 to this Annex, the substance is present in the mixture in a concentration equal to or greater than the concentration limit specified for that substance in that Appendix.
  2. For the purposes of this entry use of a mixture "for tattooing purposes" means injection or introduction of the mixture into a person's skin, mucous membrane or eyeball, by any process or procedure (including procedures commonly referred to as permanent make-up, cosmetic tattooing, micro-blading and micro-pigmentation), with the aim of making a mark or design on his or her body.
  3. If a substance not listed in Appendix 13 falls within more than one of points (a) to (g) of paragraph 1, the strictest concentration limit laid down in the points in question shall apply to that substance. If a substance listed in Appendix 13 also falls within one or more of points (a) to (g) of paragraph 1, the concentration limit laid down in point (h) of paragraph 1 shall apply to that substance.
  4. By way of derogation, paragraph 1 shall not apply to the following substances until 4 January 2023:
    - (a) Pigment Blue 15:3 (CI 74160, EC No 205-685-1, CAS No 147-14-8);
    - (b) Pigment Green 7 (CI 74260, EC No 215-524-7, CAS No 1328-53-6).
  5. If Part 3 of Annex VI to Regulation (EC) No 1272/2008 is amended after 4 January 2021 to classify or re-classify a substance such that the substance then becomes caught by point (a), (b), (c) or (d) of paragraph 1 of this entry, or such that it then falls within a different one of those points from the one within which it fell previously, and the date of application of that new or revised classification is after the date referred to in paragraph 1 or, as the case may be, paragraph 4 of this entry, that amendment shall, for the purposes of applying this entry to that substance, be treated as taking effect on the date of application of that new or revised classification.
  6. If Annex II or Annex IV to Regulation (EC) No 1223/2009 is amended after 4 January 2021 to list or change the listing of a substance such that the substance then becomes caught by point (e), (f) or (g) of paragraph 1 of this entry, or such that it then falls within a different one of those points from the one within which it fell previously, and the amendment takes effect after the date referred to in paragraph 1 or, as the case may be, paragraph 4 of this entry, that amendment shall, for the purposes of applying this entry to that substance, be treated as taking effect from the date falling 18 months after entry into force of the act by which that amendment was made.
  7. Suppliers placing a mixture on the market for use for tattooing purposes shall ensure that, after 4 January 2022, the mixture is marked with the following information:
    - (a) the statement "Mixture for use in tattoos or permanent make-up";
    - (b) a reference number to uniquely identify the batch;
    - (c) the list of ingredients in accordance with the nomenclature established in the glossary of common ingredient names pursuant to Article 33 of Regulation (EC) No 1223/2009, or in the absence of a common ingredient name, the IUPAC name. In the absence of a common ingredient name or IUPAC name, the CAS and EC number. Ingredients shall be listed in descending order by weight or volume of the ingredients at the time of formulation. "Ingredient" means any substance added during the process of formulation and present in the mixture for use for tattooing purposes. Impurities shall not be regarded as ingredients. If the name of a substance, used as ingredient within the meaning of this entry, is already required to be stated on the label in accordance with Regulation (EC) No 1272/2008, that ingredient does not need to be marked in accordance with this Regulation;
    - (d) the additional statement "pH regulator" for substances falling under point (d)(i) of paragraph 1;
    - (e) the statement "Contains nickel. Can cause allergic reactions." if the mixture contains nickel below the concentration limit specified in Appendix 13;
    - (f) the statement "Contains chromium (VI). Can cause allergic reactions." if the mixture contains chromium (VI) below the concentration limit specified in Appendix 13;
    - (g) safety instructions for use insofar as they are not already required to be stated on the label by Regulation (EC) No 1272/2008.The information shall be clearly visible, easily legible and marked in a way that is indelible. The information shall be written in the official language(s) of the Member State(s) where the mixture is placed on the market, unless the Member State(s) concerned provide(s) otherwise. Where necessary because of the size of the package, the information listed in the first subparagraph, except for point (a), shall be included instead in the instructions for use. Before using a mixture for tattooing purposes, the person using the mixture shall provide the person undergoing the procedure with the information marked on the package or included in the instructions for use pursuant to this paragraph.
  8. Mixtures that do not contain the statement "Mixture for use in tattoos or permanent make-up" shall not be used for tattooing purposes.

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

### Legend

9. This entry does not apply to substances that are gases at temperature of 20 °C and pressure of 101,3 kPa, or generate a vapour pressure of more than 300 kPa at temperature of 50 °C, with the exception of formaldehyde (CAS No 50-00-0, EC No 200-001-8).

10. This entry does not apply to the placing on the market of a mixture for use for tattooing purposes, or to the use of a mixture for tattooing purposes, when placed on the market exclusively as a medical device or an accessory to a medical device, within the meaning of Regulation (EU) 2017/745, or when used exclusively as a medical device or an accessory to a medical device, within the same meaning. Where the placing on the market or use may not be exclusively as a medical device or an accessory to a medical device, the requirements of Regulation (EU) 2017/745 and of this Regulation shall apply cumulatively.

### List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list

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 |
| E1                      | environmental hazards (hazardous to the aquatic environment, cat. 1) | 100   | 200 | 56)   |

### Notation

56) Hazardous to the Aquatic Environment in category Acute 1 or Chronic 1

### Deco-Paint Directive

|             |         |
|-------------|---------|
| VOC content | 100 %   |
| VOC content | 690 g/l |

### Industrial Emissions Directive (IED)

|             |         |
|-------------|---------|
| VOC content | 100 %   |
| VOC content | 690 g/l |

### Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

### Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

### Water Framework Directive (WFD)

not listed

### Regulation on the marketing and use of explosives precursors

not listed

### Regulation on drug precursors

not listed

### Regulation on substances that deplete the ozone layer (ODS)

not listed

### Regulation concerning the export and import of hazardous chemicals (PIC)

not listed



# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

### Regulation on persistent organic pollutants (POP)

not 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)  |
| 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

According to REACH, Article 14 (1) a chemical safety assessment has been carried out for this substance or components of this mixture when the substance has been registered in quantities of 10 tonnes or more per year per registrant.

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

## SECTION 16: Other information

### Indication of changes (revised safety data sheet)

| Section | Former entry (text/value)           | Actual entry (text/value)  | Safety-relevant |
|---------|-------------------------------------|--|-----------------|
| 2.2     |                                     | Labelling of packages where the contents do not exceed 125 ml:<br>change in the listing (table)  | yes             |
| 2.2     |                                     | Labelling of packages where the contents do not exceed 125 ml:<br>change in the listing (table)  | yes             |
| 2.3     |                                     | Endocrine disrupting properties:<br>Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.   | yes             |
| 14.8    |                                     | Regulations concerning the International Carriage of Dangerous Goods by Rail (RID)Additional information   | yes             |
| 14.8    |                                     | Classification code:<br>F1   | yes             |
| 14.8    |                                     | Danger label(s):<br>3, "Fish and tree"   | yes             |
| 14.8    |                                     | Danger label(s):<br>change in the listing (table)  | yes             |
| 14.8    |                                     | Environmental hazards:<br>Yes<br>Hazardous to water  | yes             |
| 14.8    |                                     | Excepted quantities (EQ):<br>E2  | yes             |
| 14.8    |                                     | Limited quantities (LQ):<br>1 L  | yes             |
| 14.8    |                                     | Transport category (TC):<br>2  | yes             |
| 14.8    |                                     | Hazard identification No:<br>33  | yes             |
| 15.1    | VOC content:<br>100 %<br>, 0,69 g/l | VOC content:<br>100 %  | yes             |
| 15.1    |                                     | VOC content:<br>690 g/l  | yes             |
| 15.1    | VOC content:<br>0,69 g/l            | VOC content:<br>690 g/l  | yes             |
| 15.1    |                                     | Other information:<br>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:<br>change in the listing (table)   | yes             |

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: 6889

| Section | Former entry (text/value)   | Actual entry (text/value)   | Safety-relevant |
|---------|---|---|-----------------|
| 15.2    | Chemical Safety Assessment:<br>No Chemical Safety Assessment has been carried out for this substance. | Chemical safety assessment:<br>According to REACH, Article 14 (1) a chemical safety assessment has been carried out for this substance or components of this mixture when the substance has been registered in quantities of 10 tonnes or more per year per registrant. | yes             |

### Abbreviations and acronyms

| Abbr.     | Descriptions of used abbreviations  |
|-----------|---|
| ADR       | Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)                     |
| BCF       | Bioconcentration factor   |
| 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  |
| 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  |
| EC No     | The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union) |
| 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   |
| 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   |
| 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  |
| 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)   |

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## Isooctane ROTIPURAN® ≥99,5 %, p.a., ACS

article number: **6889**

| Abbr. | Descriptions of used abbreviations  |
|-------|---|
| LL50  | Lethal Loading 50 %: the LL50 corresponds to the loading rate causing 50 % lethality  |
| NLP   | No-Longer Polymer   |
| PBT   | Persistent, Bioaccumulative and Toxic   |
| 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) |
| SVHC  | Substance of Very High Concern  |
| UEL   | Upper explosion limit (UEL)   |
| VOC   | Volatile Organic Compounds  |
| vPvB  | Very Persistent and very Bioaccumulative  |

### Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures. Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). 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.                    |
| H400 | Very toxic to aquatic life.                           |
| H410 | Very toxic to aquatic life with long lasting effects. |

### Disclaimer

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