

Safety Data Sheet

according to Regulation (EC) No 1907/2006

Isooctan mind. 99 % (2,2,4-Trimethylpentan) zur Analyse, ACS, Reag. Ph. Eur.

Revision date: 03.08.2023

Product code: 27778

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

1.1. Product identifier

Isooctan mind. 99 % (2,2,4-Trimethylpentan) zur Analyse, ACS, Reag. Ph. Eur.

REACH Registration Number: 01-2119457965-22-XXXX
CAS No: 540-84-1
Index No: 601-009-00-8
EC No: 208-759-1

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

Use of the substance/mixture

Laboratory chemicals

Industrial uses: Uses of substances as such or in preparations at industrial sites

Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Uses advised against

Do not use for private purposes (household).

1.3. Details of the supplier of the safety data sheet

Company name: AnalytiChem GmbH
Street: Stempelstraße 6
Place: D-47167 Duisburg
Telephone: 0203/5194-0
E-mail: info@analytichem.de
Contact person: Abteilung Produktsicherheit
E-mail: produktsicherheit@analytichem.de
Internet: www.analytichem.de
Responsible Department: Abteilung Produktsicherheit
Telefax: 0203/5194-290
Telephone: 0203/5194-107/117

1.4. Emergency telephone number:

For Hazardous Materials [or Dangerous Goods] Incidents Spill, Leak, Fire, Exposure, or Accident Call CHEMTREC Day or Night Within USA and Canada: 1-800-424-9300 Outside USA and Canada: +1 703-741-5970 (collect calls accepted)

Further Information

No data available

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

Flam. Liq. 2; H225
Skin Irrit. 2; H315
STOT SE 3; H336
Asp. Tox. 1; H304
Aquatic Acute 1; H400
Aquatic Chronic 1; H410

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Danger

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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. |
| H410 | Very toxic to aquatic life with long lasting effects. |

Precautionary statements

| | |
|----------------|--|
| P210 | Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. |
| P240 | Ground and bond container and receiving equipment. |
| P273 | Avoid release to the environment. |
| P301+P330+P331 | IF SWALLOWED: Rinse mouth. Do NOT induce vomiting. |
| P302+P352 | IF ON SKIN: Wash with plenty of soap and water. |
| P403+P233 | Store in a well-ventilated place. Keep container tightly closed. |

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.1. Substances

| | |
|-------------------|--------------------------------|
| Sum formula: | C ₈ H ₁₈ |
| Molecular weight: | 114.23 g/mol |

Hazardous components

| CAS No | Chemical name | Quantity | | |
|----------|---|--------------|-----------------------|-------|
| | EC No | Index No | REACH No | |
| | Classification (Regulation (EC) No 1272/2008) | | | |
| 540-84-1 | 2,2,4-trimethylpentane | | | 100 % |
| | 208-759-1 | 601-009-00-8 | 01-2119457965-22-XXXX | |
| | Flam. Liq. 2, Skin Irrit. 2, STOT SE 3, Asp. Tox. 1, Aquatic Acute 1, Aquatic Chronic 1; H225 H315 H336 H304 H400 H410 | | | |

Full text of H and EUH statements: see section 16.

Specific Conc. Limits, M-factors and ATE

| CAS No | EC No | Chemical name | Quantity |
|----------|---|------------------------|----------|
| | Specific Conc. Limits, M-factors and ATE | | |
| 540-84-1 | 208-759-1 | 2,2,4-trimethylpentane | 100 % |
| | inhalation: LC ₅₀ = > 33,52 mg/l (vapours); dermal: LD ₅₀ = > 2000 mg/kg; oral: LD ₅₀ = > 5000 mg/kg | | |

Further Information

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of = 0.1 % (w/w).

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

No data available

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After inhalation

Provide fresh air.
Call a physician immediately.

After contact with skin

Wash immediately with: Water
Take off immediately all contaminated clothing and wash it before reuse.

After contact with eyes

Rinse immediately carefully and thoroughly with eye-bath or water.
Remove contact lenses, if present and easy to do. Continue rinsing.

After ingestion

Observe risk of aspiration if vomiting occurs.
Call a physician immediately.

4.2. Most important symptoms and effects, both acute and delayed

Irritant
Vapours may cause drowsiness and dizziness.
Narcotic effects
Pulmonary oedema

4.3. Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂)
Foam
Extinguishing powder

Unsuitable extinguishing media

no restriction

5.2. Special hazards arising from the substance or mixture

Combustible liquids
Hazardous combustion products
In case of fire may be liberated: Carbon dioxide (CO₂) Carbon monoxide
Vapours are heavier than air, spread along floors and form explosive mixtures with air.
Heating causes rise in pressure with risk of bursting.
Beware of reignition.

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.
In case of fire and/or explosion do not breathe fumes.
Avoid contact with skin, eyes and clothes.

Additional information

Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.
Move undamaged containers from immediate hazard area if it can be done safely.
Use water spray jet to protect personnel and to cool endangered containers.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General advice

Keep away from sources of ignition - No smoking.
This material can be ignited by heat, sparks, flames, or other sources of ignition (e.g., static electricity, pilot lights, mechanical/electrical equipment, and electronic devices such as cell phones, computers, calculators,

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and pagers which have not been certified as intrinsically safe).

Take action to prevent static discharges.

For non-emergency personnel

Provide adequate ventilation.

Use personal protection equipment.

Avoid contact with skin, eyes and clothes.

Remove persons to safety.

Emergency procedures

Do not breathe dust/fume/gas/mist/vapours/spray.

For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

The vapour of the product is heavier than air and may accumulate below ground level, in pits, channels and basements in higher concentration.

Danger of explosion

6.3. Methods and material for containment and cleaning up

For containment

Cover drains.

Prevent spread over a wide area (e.g. by containment or oil barriers).

Collect in closed and suitable containers for disposal.

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

For cleaning up

Clean contaminated articles and floor according to the environmental legislation.

Other information

Provide adequate ventilation.

Do not breathe dust/fume/gas/mist/vapours/spray.

Wear breathing apparatus if exposed to vapours/dusts/aerosols.

6.4. Reference to other sections

Safe handling: see section 7

Personal protection equipment: see section 8

Disposal: see section 13

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

Read label before use. Handle and open container with care.

When using do not eat, drink, smoke, sniff. Keep container tightly closed.

Use personal protection equipment. Use extractor hood (laboratory).

Provide adequate ventilation. Do not breathe vapour.

Advice on protection against fire and explosion

Take action to prevent static discharges. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.

Further information on handling

Take off immediately all contaminated clothing and wash it before reuse.

Draw up and observe skin protection programme. Wash hands and face before breaks and after work and take a shower if necessary. If handled uncovered, arrangements with local exhaust ventilation have to be used.

7.2. Conditions for safe storage, including any incompatibilities

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Requirements for storage rooms and vessels

Keep in a cool, well-ventilated place.

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

Further information on storage conditions

Keep container tightly closed and dry.

Keep cool. Protect from sunlight.

storage temperature +5°C - +30°C

7.3. Specific end use(s)

Laboratory chemicals

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

DNEL/DMEL values

| CAS No | Substance | Exposure route | Effect | Value |
|--------------------------|------------------------|----------------|----------|------------------------|
| 540-84-1 | 2,2,4-trimethylpentane | | | |
| Worker DNEL, long-term | | inhalation | systemic | 2035 mg/m ³ |
| Worker DNEL, long-term | | dermal | systemic | 773 mg/kg bw/day |
| Consumer DNEL, long-term | | inhalation | systemic | 608 mg/m ³ |
| Consumer DNEL, long-term | | dermal | systemic | 699 mg/kg bw/day |
| Consumer DNEL, long-term | | oral | systemic | 699 mg/kg bw/day |

8.2. Exposure controls

Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection equipment.

If handled uncovered, arrangements with local exhaust ventilation have to be used.

Individual protection measures, such as personal protective equipment

Eye/face protection

goggles

Face protection umbrella

Hand protection

Protective gloves are recommended Company KCL GmbH, D-36124 Eichenzell, email: vertrieb@kcl.de With specification (test according to EN374):

By long-term hand contact

Trade name/designation KCL 730 Camatril® Velours

Suitable material: NBR (Nitrile rubber) 0,4 mm

Wearing time with permanent contact: > 480 min

By short-term hand contact

Trade name/designation KCL 741 Dermatril® L

Suitable material: NBR (Nitrile rubber) 0,11 mm

Wearing time with occasional contact (splashes): > 60 min

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types. This recommendation applies only to the product stated in the safety data sheet (>,<) supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves

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(e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Skin protection

- Take off immediately all contaminated clothing and wash it before reuse.
- Wear fire resistant or flame retardant clothing.
- Wash hands and face before breaks and after work and take a shower if necessary.
- Draw up and observe skin protection programme.

Respiratory protection

- Wear breathing apparatus if exposed to vapours/dusts/aerosols.
- Filtering device with filter or ventilator filtering device of type: A

Environmental exposure controls

- Do not allow to enter into surface water or drains.
- Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches.
- Danger of explosion

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

| | |
|---|------------------------|
| Physical state: | Liquid |
| Colour: | colourless |
| Odour: | like: Gasoline |
| Odour threshold: | No data available |
| Melting point/freezing point: | -107 °C |
| Boiling point or initial boiling point and boiling range: | 99 °C |
| Flammability: | No data available |
| Lower explosion limits: | 1 vol. % |
| Upper explosion limits: | 6 vol. % |
| Flash point: | -12 °C |
| Auto-ignition temperature: | 418 °C |
| Decomposition temperature: | No data available |
| pH-Value: | No data available |
| Viscosity / kinematic: | No data available |
| Water solubility: (at 25 °C) | 0,56 g/L |
| Solubility in other solvents | No data available |
| Dissolution rate: | No data available |
| Partition coefficient n-octanol/water: | log Pow: 4,09 |
| Dispersion stability: | No data available |
| Vapour pressure: (at 20 °C) | 51 hPa |
| Vapour pressure: | No data available |
| Density: | 0,69 g/cm ³ |
| Relative density: | No data available |
| Bulk density: | No data available |
| Relative vapour density: | No data available |
| Particle characteristics: | No data available |

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

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

Sustaining combustion: Sustaining combustion

Self-ignition temperature

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| | |
|-------------------------------------|-------------------|
| Solid: | No data available |
| Gas: | No data available |
| Oxidizing properties | |
| No data available | |
| Other safety characteristics | |
| Evaporation rate: | No data available |
| Solvent separation test: | No data available |
| Solvent content: | 100% |
| Solid content: | No data available |
| Sublimation point: | No data available |
| Softening point: | No data available |
| Pour point: | No data available |
| Viscosity / dynamic: (at 20 °C) | 0,5 mPa·s |
| Flow time: | No data available |

Further Information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

Vapours may form explosive mixtures with air.

10.2. Chemical stability

The product is stable under storage at normal ambient temperatures.

10.3. Possibility of hazardous reactions

Oxidising agent

10.4. Conditions to avoid

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

10.5. Incompatible materials

Plastic articles

10.6. Hazardous decomposition products

SECTION 5: Firefighting measures

Further information

No data available

SECTION 11: Toxicological information

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

Toxicokinetics, metabolism and distribution

No data available

Acute toxicity

Based on available data, the classification criteria are not met.

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| CAS No | Chemical name | | | | |
|----------|-------------------------|-------------------|---------|---------------------|--------------------|
| | Exposure route | Dose | Species | Source | Method |
| 540-84-1 | 2,2,4-trimethylpentane | | | | |
| | oral | LD50 > 5000 mg/kg | Rat | Study report (1982) | OECD Guideline 401 |
| | dermal | LD50 > 2000 mg/kg | Rabbit | Study report (1982) | OECD Guideline 402 |
| | inhalation (4 h) vapour | LC50 > 33,52 mg/l | Rat | Study report (1982) | OECD Guideline 403 |

Irritation and corrosivity

Causes skin irritation.

Serious eye damage/eye irritation: Based on available data, the classification criteria are not met.

Prolonged or repeated skin contact may cause removal of natural fat from the skin resulting in dermatitis (skin inflammation).

Sensitising effects

Based on available data, the classification criteria are not met.

Carcinogenic/mutagenic/toxic effects for reproduction

Based on available data, the classification criteria are not met.

STOT-single exposure

May cause drowsiness or dizziness. (2,2,4-trimethylpentane)

Organs affected: central nervous system

STOT-repeated exposure

Based on available data, the classification criteria are not met.

Aspiration hazard

May be fatal if swallowed and enters airways.

Information on likely routes of exposure

No data available

Specific effects in experiment on an animal

No data available

Additional information on tests

No data available

Practical experience

No data available

11.2. Information on other hazards

Endocrine disrupting properties

No data available

Other information

No data available

Further information

Irritant

Vapours may cause drowsiness and dizziness.

Narcotic effects

Pulmonary oedema

SECTION 12: Ecological information

12.1. Toxicity

Very toxic to aquatic life.

Very toxic to aquatic life with long lasting effects.

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| CAS No | Chemical name | | | | | | |
|----------|--------------------------|---------------|-----------|---------|---------------------------------|---|--|
| | Aquatic toxicity | Dose | [h] [d] | Species | Source | Method | |
| 540-84-1 | 2,2,4-trimethylpentane | | | | | | |
| | Acute fish toxicity | LC50 mg/l | 0,11 | 96 h | Oncorhynchus mykiss | SIDS Initial Assessment Report For SIAM | OECD Guideline 203 |
| | Acute algae toxicity | ErC50 mg/l | 2,943 | 72 h | Pseudokirchneriella subcapitata | CONCAWE, Brussels, Belgium (2010) | The aquatic toxicity was estimated by a |
| | Acute crustacea toxicity | EC50 | 0,4 mg/l | 48 h | Daphnia magna | Publication (1986) | other: As described in: The evaluation o |
| | Fish toxicity | NOEC mg/l | 0,82 | 28 d | Oncorhynchus mykiss | CONCAWE, Brussels, Belgium (2010) | The aquatic toxicity was estimated by a |
| | Crustacea toxicity | NOEC | 1 mg/l | 21 d | Daphnia magna | SIDS Initial Assessment Report For SIAM | OECD Guideline 211 |

12.2. Persistence and degradability

No data available

12.3. Bioaccumulative potential

Bioaccumulative potential

Partition coefficient n-octanol/water

| CAS No | Chemical name | Log Pow |
|----------|------------------------|---------|
| 540-84-1 | 2,2,4-trimethylpentane | 4,08 |

BCF

| CAS No | Chemical name | BCF | Species | Source |
|----------|------------------------|-----|------------|----------------------|
| 540-84-1 | 2,2,4-trimethylpentane | 231 | calculated | Other company data (|

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

12.7. Other adverse effects

Do not allow to enter into surface water or drains.

Avoid release to the environment.

Further information

No data available

SECTION 13: Disposal considerations**13.1. Waste treatment methods****Disposal recommendations**

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.

Send to a physico-chemical treatment facility under observation of official regulations.

Do not empty into drains.

Contaminated packaging

Handle contaminated packages in the same way as the substance itself.

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

SECTION 14: Transport information

Land transport (ADR/RID)

| | |
|--|---------|
| 14.1. UN number or ID number: | UN 1262 |
| 14.2. UN proper shipping name: | OCTANES |
| 14.3. Transport hazard class(es): | 3 |
| 14.4. Packing group: | II |
| Hazard label: | 3 |
| Classification code: | F1 |
| Limited quantity: | 1 L |
| Excepted quantity: | E2 |
| Transport category: | 2 |
| Hazard No: | 33 |
| Tunnel restriction code: | D/E |

Inland waterways transport (ADN)

| | |
|--|---------|
| 14.1. UN number or ID number: | UN 1262 |
| 14.2. UN proper shipping name: | OCTANES |
| 14.3. Transport hazard class(es): | 3 |
| 14.4. Packing group: | II |
| Hazard label: | 3 |
| Classification code: | F1 |
| Limited quantity: | 1 L |
| Excepted quantity: | E2 |

Marine transport (IMDG)

| | |
|--|----------|
| 14.1. UN number or ID number: | UN 1262 |
| 14.2. UN proper shipping name: | OCTANES |
| 14.3. Transport hazard class(es): | 3 |
| 14.4. Packing group: | II |
| Hazard label: | 3 |
| Marine pollutant: | P |
| Special Provisions: | - |
| Limited quantity: | 1 L |
| Excepted quantity: | E2 |
| EmS: | F-E, S-E |

Air transport (ICAO-TI/IATA-DGR)

| | |
|--|---------|
| 14.1. UN number or ID number: | UN 1262 |
| 14.2. UN proper shipping name: | OCTANES |
| 14.3. Transport hazard class(es): | 3 |
| 14.4. Packing group: | II |
| Hazard label: | 3 |
| Limited quantity Passenger: | 1 L |
| Passenger LQ: | Y341 |
| Excepted quantity: | E2 |
| IATA-packing instructions - Passenger: | 353 |
| IATA-max. quantity - Passenger: | 5 L |
| IATA-packing instructions - Cargo: | 364 |
| IATA-max. quantity - Cargo: | 60 L |

14.5. Environmental hazards

| | |
|-----------------------------|--------|
| ENVIRONMENTALLY HAZARDOUS: | Yes |
| Danger releasing substance: | octane |

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SECTION 15: Regulatory information

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

EU regulatory information

Restrictions on use (REACH, annex XVII):

Entry 3, Entry 40, Entry 75

Information according to 2012/18/EU
(SEVESO III):

E1 Hazardous to the Aquatic Environment

Additional information:

P5c

National regulatory information

Employment restrictions:

Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC).

Water hazard class (D):

2 - obviously hazardous to water

15.2. Chemical safety assessment

For this substance a chemical safety assessment is not required.

SECTION 16: Other information

Changes

This data sheet contains changes from the previous version in section(s): 12.

Abbreviations and acronyms

Flam. Liq: Flammable liquid

Asp. Tox: Aspiration hazard

Skin Irrit: Skin irritation

STOT SE: Specific target organ toxicity - single exposure

Aquatic Acute: Acute aquatic hazard

Aquatic Chronic: Chronic aquatic hazard

Relevant H and EUH statements (number and full 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.

Further Information

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. The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights.

The receiver of our product is singularly responsible for adhering to existing laws and regulations.