SAFETY DATA SHEET

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

1.1 Product identifiers

Product name : 2,2,4-Trimethylpentane

Product Number : 360066
Brand : Sigma-Aldrich
Index-No. : 601-009-00-8
CAS-No. : 540-84-1

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO  63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

- Flammable liquids (Category 2), H225
- Skin irritation (Category 2), H315
- Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336
- Aspiration hazard (Category 1), H304
- Short-term (acute) aquatic hazard (Category 1), H400
- Long-term (chronic) aquatic hazard (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram
Signal Word | Danger
---|---
Hazard statement(s) | Highly flammable liquid and vapor.
  | May be fatal if swallowed and enters airways.
  | Causes skin irritation.
  | May cause drowsiness or dizziness.
  | Very toxic to aquatic life with long lasting effects.
Precautionary statement(s) | Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
  | Keep container tightly closed.
  | Ground/bond container and receiving equipment.
  | Use explosion-proof electrical/ ventilating/ lighting/ equipment.
  | Use only non-sparking tools.
  | Take precautionary measures against static discharge.
  | Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
  | Wash skin thoroughly after handling.
  | Use only outdoors or in a well-ventilated area.
  | Avoid release to the environment.
  | Wear protective gloves/ eye protection/ face protection.
  | IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
  | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
  | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
  | Do NOT induce vomiting.
  | If skin irritation occurs: Get medical advice/ attention.
  | Take off contaminated clothing and wash before reuse.
  | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
  | Collect spillage.
  | Store in a well-ventilated place. Keep container tightly closed.
  | Store in a well-ventilated place. Keep cool.
  | Store locked up.
  | Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances
Synonyms | Isooctane
---|---
Formula | C₈H₁₈
Molecular weight | 114.23 g/mol
CAS-No. | 540-84-1
EC-No. | 208-759-1
Index-No. | 601-009-00-8

| Component | Classification | Concentration |
isooctane

| Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H315, H336, H304, H400, H410 | <= 100 % |
| Concentration limits: >= 20 %: STOT SE 3, H336; M-Factor - Aquatic Acute: 10 M-Factor - Aquatic Chronic: 1 |

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air. Call in physician.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower.

In case of eye contact
After eye contact: rinse out with plenty of water. Remove contact lenses.

If swallowed

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

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 Dry powder

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.
5.2 **Special hazards arising from the substance or mixture**
Carbon oxides
Flash back possible over considerable distance. Container explosion may occur under fire conditions.
Combustible.
Pay attention to flashback.
Vapors are heavier than air and may spread along floors.
Development of hazardous combustion gases or vapours possible in the event of fire.
Forms explosive mixtures with air at ambient temperatures.

5.3 **Advice for firefighters**
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 **Further information**
Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

---

**SECTION 6: Accidental release measures**

6.1 **Personal precautions, protective equipment and emergency procedures**
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.
Evacuate the danger area, observe emergency procedures, consult an expert.
For personal protection see section 8.

6.2 **Environmental precautions**
Do not let product enter drains. Risk of explosion.

6.3 **Methods and materials for containment and cleaning up**
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 **Reference to other sections**
For disposal see section 13.

---

**SECTION 7: Handling and storage**

7.1 **Precautions for safe handling**

**Advice on safe handling**
Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

**Advice on protection against fire and explosion**
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

**Hygiene measures**
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
For precautions see section 2.2.

7.2 **Conditions for safe storage, including any incompatibilities**

**Storage conditions**
Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

**Storage class**
Storage class (TRGS 510): 3: Flammable liquids

### 7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

---

### SECTION 8: Exposure controls/personal protection

#### 8.1 Control parameters

**Ingredients with workplace control parameters**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>isooctane</td>
<td>540-84-1</td>
<td>TWA</td>
<td>300 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
</tbody>
</table>

#### 8.2 Exposure controls

**Appropriate engineering controls**
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

**Personal protective equipment**

**Eye/face protection**
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

**Skin protection**
required

**Body Protection**
Flame retardant antistatic protective clothing.

**Respiratory protection**
required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

**Control of environmental exposure**
Do not let product enter drains. Risk of explosion.

---

### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

a) **Appearance**
   Form: liquid
   Color: colorless

b) **Odor**
   No data available

c) **Odor Threshold**
   No data available

d) **pH**
   No data available

e) **Melting**
   Melting point/range: -107 °C (-161 °F)
<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Freezing point</td>
<td>98 - 99 °C 208 - 210 °F</td>
</tr>
<tr>
<td>Initial boiling point and boiling range</td>
<td>-12 °C (10 °F) - closed cup</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>Upper/lower flammability or explosive limits</td>
<td>Upper explosion limit: 6 % (V)</td>
</tr>
<tr>
<td></td>
<td>Lower explosion limit: 1 % (V)</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>55 hPa at 21 °C (70 °F)</td>
</tr>
<tr>
<td></td>
<td>120 hPa at 37.80 °C (100.04 °F)</td>
</tr>
<tr>
<td>Vapor density</td>
<td>3.94 - (Air = 1.0)</td>
</tr>
<tr>
<td>Density</td>
<td>0.692 g/mL at 25 °C (77 °F)</td>
</tr>
<tr>
<td>Relative density</td>
<td>No data available</td>
</tr>
<tr>
<td>Water solubility</td>
<td>insoluble</td>
</tr>
<tr>
<td>Partition coefficient: n-octanol/water</td>
<td>log Pow: 4.6 - Bioaccumulation is not expected.</td>
</tr>
<tr>
<td>Autoignition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Viscosity</td>
<td>No data available</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td>Oxidizing properties</td>
<td>none</td>
</tr>
</tbody>
</table>

**9.2 Other safety information**

- Relative vapor density: 3.94 - (Air = 1.0)

**SECTION 10: Stability and reactivity**

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions

Violent reactions possible with:
- Strong oxidizing agents

10.4 Conditions to avoid

Warming.
10.5 **Incompatible materials**
Various plastics

10.6 **Hazardous decomposition products**
In the event of fire: see section 5

**SECTION 11: Toxicological information**

**11.1 Information on toxicological effects**

**Acute toxicity**
LD50 Oral - Rat - male and female - > 5,000 mg/kg
(OECD Test Guideline 401)
LC50 Inhalation - Rat - male and female - 4 h - > 33.52 mg/l - vapor

(OECD Test Guideline 403)
Symptoms: mucosal irritations
LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

**Skin corrosion/irritation**
Skin - Rabbit
Result: Irritating to skin. - 24 h
(OECD Test Guideline 404)
Remarks: Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

**Serious eye damage/eye irritation**
Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)

**Respiratory or skin sensitization**
Maximization Test - Guinea pig
Result: negative
(OECD Test Guideline 406)

**Germ cell mutagenicity**
Test Type: Ames test
Test system: TA98
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative
Test Type: In vitro mammalian cell gene mutation test
Test system: human lymphoblastoid cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative

Test Type: unscheduled DNA synthesis assay
Species: Rat
Cell type: Liver cells
Application Route: Oral
Method: OECD Test Guideline 486
Result: negative

**Carcinogenicity**
IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA’s list of regulated carcinogens.

**Reproductive toxicity**
No data available

**Specific target organ toxicity - single exposure**
May cause drowsiness or dizziness. - Central nervous system

**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

### 11.2 Additional Information

RTECS: SA3320000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

It generally applies for aliphatic hydrocarbons with 6 - 18 carbon atoms that they may cause pneumonia, in some cases also pulmonary oedema, upon direct inhalation, i.e. in conditions that can occur only in very special circumstances (nebulizations, spraying, inhalation of aerosols and similar). After absorption of very large quantities: narcosis.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Liver - Irregularities - Based on Human Evidence

Liver - Irregularities - Based on Human Evidence

### SECTION 12: Ecological information

#### 12.1 Toxicity

**Toxicity to fish**
semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) - 0.11 mg/l - 96 h
(OECD Test Guideline 203)

**Toxicity to daphnia and other aquatic invertebrates**
static test EC50 - Daphnia magna (Water flea) - 0.4 mg/l - 48 h
Remarks: (in analogy to similar products)
(ECHA)
The value is given in analogy to the following substances: 2,3,4-Trimethylpentane

**Toxicity to bacteria**
EC0 - Pseudomonas putida - 10,000 mg/l
Remarks: (IUCLID)
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)

12.2 Persistence and degradability

Biodegradability: aerobic - Exposure time 28 d
Result: 51.3 % - Inherently biodegradable. (OECD Test Guideline 301F)

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

Biological effects:
Endangers drinking-water supplies if allowed to enter soil and/or waters in large quantities. Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)
UN number: 1262 Class: 3 Packing group: II
Proper shipping name: Octanes
Reportable Quantity (RQ): 1000 lbs
Marine pollutant: yes Poison Inhalation Hazard: No

IMDG
UN number: 1262 Class: 3 Packing group: II EMS-No: F-E, S-E
Proper shipping name: OCTANES
Marine pollutant: yes
Marine pollutant: yes
**IATA**
UN number: 1262   Class: 3   Packing group: II
Proper shipping name: Octanes

---

**SECTION 15: Regulatory information**

**SARA 302 Components**
This material does not contain any components with a section 302 EHS TPQ.

**SARA 313 Components**
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>isooctane</td>
<td>540-84-1</td>
<td>2007-03-01</td>
</tr>
</tbody>
</table>

**Pennsylvania Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>isooctane</td>
<td>540-84-1</td>
<td>2007-03-01</td>
</tr>
</tbody>
</table>

**New Jersey Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>isooctane</td>
<td>540-84-1</td>
<td>2007-03-01</td>
</tr>
</tbody>
</table>
SECTION 16: Other information

Further information
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.
The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 6.7  Revision Date: 03/18/2023  Print Date: 08/12/2023