

# SAFETY DATA SHEET

## Trimethylpentane, 2,2,4- (ISOOCTANE)

This SDS is valid for all grades that start with catalog number  
398

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### 1. IDENTIFICATION OF SUBSTANCE / MIXTURE AND OF SUPPLIER

**Product Identifier:** High Purity Chemicals  
**Synonyms:** Isooctane Isobutyltrimethylmethane  
**Other means of identification:** CAS No. 540-84-1  
EINECS No. 208-759-1

**Recommended use of the chemical and restrictions on use:**

**Supplier Details:**

**Pharmco Products, Inc.**  
58 Vale Road, Brookfield,  
CT 06804, USA.  
Tel: 203.740.3471  
Fax: 203.740.3481  
CCN17213

**Emergency Contact:** CHEMTREC: 1.800.424.9300 (USA) / +1.703.527.3887 (International)

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### 2. HAZARDS IDENTIFICATION

**OSHA Hazards:**

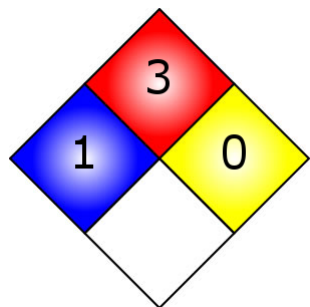
Flammable liquid, Target Organ Effect, Irritant, Harmful by ingestion, Harmful by skin absorption

**Target Organs:**

Blood, Central nervous system, Kidney, Liver, Lungs

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**NFPA**



**GHS label elements, including precautionary statements**



**Signal Word:**  
DANGER!

**Hazard statement(s)**

H225	Highly flammable liquid and vapor.
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 statement(s)**

P210	Keep away from heat, sparks, open flames, and hot surfaces. No smoking.
P241	Use explosion-proof electrical, ventilating, and lighting equipment.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER or a doctor/physician.
P303 + P361 + P353	IF ON SKIN (or hair): Remove immediately all contaminated clothing. Rinse skin with water.
P405	Store locked up.
P501	Dispose of contents and container to an approved waste disposal plant.

**GHS Classification(s)**

Skin irritation (Category 2)  
Aspiration hazard (Category 1)  
Specific target organ toxicity - single exposure (Category 3)

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Chronic aquatic toxicity (Category 1)

Flammable Liquids (Category 2)

**Other hazards which do not result in classification:**

**Potential Health Effects:**

Organ	Description
Eyes	Causes eye irritation.
Ingestion	May be harmful if swallowed.
Inhalation	May be harmful if inhaled. Causes respiratory tract irritation. Vapors may cause drowsiness and dizziness.
Skin	Harmful if absorbed through skin. Causes skin irritation.

### 3. COMPOSITION AND INFORMATION ON INGREDIENTS

<b>Chemical identity:</b>	2,2,4-Trimethylpentane
<b>Common name / Synonym:</b>	Isooctane Isobutyltrimethylmethane
<b>CAS number:</b>	540-84-1
<b>EINECS number:</b>	208-759-1
<b>ICSC number:</b>	0496
<b>RTECS #:</b>	SA3320000
<b>UN #:</b>	1262
<b>EC #:</b>	601-009-00-8

% Weight	Material	CAS
100	ISOOCTANE (2,2,4-TRIMETHYLPENTANE)	540-81-1

### 4. FIRST AID MEASURES

#### General advice

Take proper precautions to ensure your own health and safety before attempting rescue and providing first aid.  
Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### Skin

Wash skin with soap and copious amounts of water. Seek medical attention.

#### Inhalation

Remove person to fresh air. If signs/symptoms continue, get medical attention. Give oxygen or artificial respiration as needed.

#### Eyes

Flush eyes with water as a precaution.

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#### **Ingestion**

DO NOT induce vomiting. If vomiting does occur, have victim lean forward to prevent aspiration. Rinse mouth with water. Seek medical attention. Never give anything by mouth to an unconscious individual.

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## **5. FIRE FIGHTING MEASURES**

#### **Suitable (and unsuitable) extinguishing media:**

SMALL FIRE: Use dry chemicals, CO<sub>2</sub>, water spray or alcohol-resistant foam. LARGE FIRE: Use water spray, water fog or alcohol-resistant foam. Cool all affected containers with flooding quantities of water.

#### **Specific hazards arising from the chemical (e.g., nature of any hazardous combustion products):**

Flash back possible over considerable distance. Container explosion may occur under fire conditions.

#### **Special protective equipment and precautions for firefighters:**

Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes. Keep unopened containers cool by spraying with water.

#### **Unusual Fire and Explosion Hazards:**

- Extremely flammable

EXTREMELY FLAMMABLE. EVACUATE A RADIUS OF 1500 FEET FOR UNCONTROLLABLE FIRES. CONSIDER EVACUATION DOWNWIND IF MATERIAL IS LEAKING.

#### **Flammable Properties**

##### **Classification**

OSHA/NFPA Class IB Flammable Liquid.

##### **Flash point**

-12°C (10°F)

##### **Autoignition temperature**

415°C (779°F)

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## **6. ACCIDENTAL RELEASE MEASURES**

#### **Personal precautions, protective equipment and emergency procedures:**

Do not inhale vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

#### **Environmental precautions:**

Stop leak. Contain spill if possible and safe to do so. Prevent product from entering drains.

#### **Methods and materials for containment and cleaning up:**

Highly flammable liquid. Eliminate all sources of ignition. All equipment used when handling this product must be

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grounded. A vapor suppressing foam may be used to reduce vapors. Do not touch or walk through spilled material. Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations. Use clean non-sparking tools to collect absorbed material.

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## 7. HANDLING AND STORAGE

### Precautions for safe handling:

Do not get on skin or in eyes. Do not inhale vapor or mist. Keep away from sources of ignition - No smoking. Take measures to prevent the buildup of electrostatic charge. Open and handle container with care. Metal containers involved in the transfer of this material should be grounded and bonded.

### Conditions for safe storage, including any incompatibilities:

Store in a closed container in a cool, dry, well-ventilated area. Keep containers upright and tightly closed to prevent leaks/spills.

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## 8. EXPOSURE CONTROLS / PERSONAL PROTECTION

### Control parameters, e.g., occupational exposure limit values or biological limit values:

#### Occupational Exposure Limits

Component	Source	Type	Value	Note
2,2,4-Trimethylpentane	/		No exposure limit	

### Appropriate engineering controls:

General room or local exhaust ventilation is usually required to meet exposure limit(s). Electrical equipment should be grounded and conform to applicable electrical code.

### Individual protection measures, such as personal protective equipment:

#### Respiratory protection:

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### Hand protection:

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

#### Eye protection:

Use chemical safety goggles and/or a full face shield where splashing is possible. Use equipment approved by appropriate government standards, such as NIOSH (US) or EN166 (EU) Maintain eye wash fountain and

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quick-drench facilities in work area.

**Skin and body protection:**

Wear impervious protective clothing, including boots, gloves, lab coat, apron or coveralls, as appropriate, to prevent skin contact.

**Hygiene measures:**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

<b>Appearance (physical state, color, etc.)</b>	Clear colorless liquid
<b>Odor</b>	Gasoline-like
<b>Freezing point</b>	-107 °C (-161 °F)
<b>Initial boiling point and boiling range</b>	98 - 99 °C (208 - 211 °F)
<b>Flash point</b>	-12 °C (10 °F) - closed cup
<b>Upper / Lower flammability or explosive limits</b>	1 %(V) / 6 %(V)
<b>Vapor pressure</b>	55 hPa (41 mmHg) at 21 °C (70 °F) 117 hPa (88 mmHg) at 37.80 °C (100.04 °F)
<b>Vapor Density</b>	3.9 (AIR=1)
<b>Solubility(ies)</b>	Negligible
<b>Partition coefficient n-octanol/water(ies)</b>	log Pow: 4.6
<b>Auto-ignition temperature</b>	415°C (779°F)
<b>Formula (2,2,4-TRYMETHYLPENTANE)</b>	C <sub>8</sub> H <sub>18</sub>
<b>Molecular Formula (2,2,4-TRIMETHYLPENTANE)</b>	114.23 g/mol

## 10. STABILITY AND REACTIVITY

<b>Chemical Stability</b>	Stable under recommended storage conditions.
<b>Possibility of hazardous reactions</b>	Vapors may form explosive mixture with air.
<b>Conditions to avoid (e.g., static discharge, shock or vibration)</b>	Heat, flames, and sparks. Extreme temperatures and direct sunlight.
<b>Incompatible materials</b>	Strong oxidizing agents
<b>Hazardous decomposition products</b>	Hazardous decomposition products formed under fire conditions. - Carbon oxides

## 11. TOXICOLOGICAL INFORMATION

- 2,2,4-Trimethylpentane 540-84-1

**Product Summary:**

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No data available for the teratogenic, or reproductive toxicity effects of this product. Lab tests have shown genotoxicity in vivo.

**Acute Toxicity:**

LD50 (Oral)	Rat	> 5000 mg/kg	
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**Aspiration Hazard (2,2,4-TRIMETHYLPENTANE)**

The substance or mixture is known to cause human aspiration toxicity hazards or has to be regarded as if it causes a human aspiration toxicity hazard

**Carcinogenicity**

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

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

**Other Hazards**

Organ	Description
Eyes	Causes eye irritation.
Ingestion	May be harmful if swallowed.
Inhalation	May be harmful if inhaled. Causes respiratory tract irritation. Vapors may cause drowsiness and dizziness.
Skin	Harmful if absorbed through skin. Causes skin irritation.

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## 12. ECOLOGICAL INFORMATION

- 2,2,4-Trimethylpentane 540-84-1

**Other adverse effects:**

An environmental hazard is possible if product is handled or disposed of improperly. Product is highly toxic to aquatic life with long term effects.

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## 13. DISPOSAL CONSIDERATIONS

Description of waste residues and information on their safe handling and methods of disposal, including the

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**disposal of any contaminated packaging:**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Observe all federal, state, and local environmental regulations. Contact a licensed professional waste disposal service to dispose of this material.

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## 14. TRANSPORT INFORMATION

**Description of waste residues and information on their safe handling and methods of disposal:**

<b>UN number</b>	1262
<b>UN proper shipping name</b>	Octanes
<b>Transport hazard class(es)</b>	3
<b>Packing group (if applicable)</b>	II

**Reportable Quantity**

1,000 lbs.

**IMDG**

UN-Number: 1262 Class: 3 Packing Group: II

EMS-No: F-E, S-E

Proper shipping name: OCTANES

Marine pollutant: No

**IATA**

UN-Number: 1262 Class: 3 Packing Group: II

Proper shipping name: Octanes

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## 15. REGULATORY INFORMATION

**Safety, health and environmental regulations specific for the product in question:**

**OSHA Hazards**

Flammable liquid, Target Organ Effect, Irritant, Harmful by ingestion, Harmful by skin absorption

All ingredients are on the following inventories or are exempted from listing

<b>Country</b>	<b>Notification</b>
Australia	AICS
Canada	DSL
China	IECS
European Union	EINECS
Japan	ENCS/ISHL
Korea	ECL
New Zealand	NZIoC
Philippines	PICCS
United States of America	TSCA

**SARA 302 Components**



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No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**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**

Acute Health Hazard

Chronic Health Hazard

Fire Hazard

**Massachusetts Right To Know Components**

2,2,4-Trimethylpentane CAS-No. 540-84-1 Revision Date 2007-03-01

**Pennsylvania Right To Know Components**

2,2,4-Trimethylpentane CAS-No. 540-84-1 Revision Date 2007-03-01

**New Jersey Right To Know Components**

2,2,4-Trimethylpentane CAS-No. 540-84-1 Revision Date 2007-03-01

**California Prop 65 Components**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## **16. OTHER INFORMATION: INCLUDING INFORMATION ON PREPARATION AND REVISION OF THE SDS**

**Disclaimer**

PHARMCO-AAPER believes that the information on this SDS was obtained from reliable sources. However, the information is provided without any warranty, expressed or implied, regarding its correctness. Some information presented and conclusions drawn herein are from sources other than direct test data on the substance itself. The conditions or methods of handling, storage, use and disposal of the product are beyond our control and may be beyond our knowledge. For this and other reasons, PHARMCO-AAPER does not assume responsibility and expressly disclaims liability for loss, damage, or expense arising out of or in any way connected with handling, storage, use, or disposal of this product. If the product is used as a component in another product, this SDS information may not be applicable. Information is correct to the best of our knowledge at the date of the SDS publication.