

Material Safety Data Sheet



2,2,4-TRIMETHYLPENTANE FOR HPLC
(iso-Octane)

VERSION : 05
REVISION DATE : 14/06/2025
EFFECTIVE DATE : 16/06/2025

Product Code : 42900

Page 1 of 14

1. Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Trade name : **2,2,4-TRIMETHYLPENTANE FOR HPLC**
Product code : 42900
Identification of the product : 2,2,4-TRIMETHYLPENTANE FOR HPLC
CAS No : 540-84-1
EC Index-No. : 601-009-00-8
EC No. : 208-759-1
Synonyms : iso-Octane

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

Identified uses : Laboratory chemicals, Manufacture of substances

1.3. Details of the supplier of the safety data sheet

Company identification

MOLYCHEM INDIA LLP
Office: Maker Tower 'E', 41-A2, 4th Floor, Above Maker
Arcade, Cuffe Parade, Mumbai 400 005 (INDIA)
Tel: +91 22 4066 8111, 2205 7772 .
Email : info@molychem.net
Works: Plot No. B/9, Badlapur M.I.D.C.,
OPP.Shobhavat Textile Co., Kulgaon, Badlapur (E),
Dist.-Thane-421 503.

1.4. Emergency telephone number

Emergency number : +91 22 4066 8111 (10:00am - 6:00 pm)

2. Hazards identification

2.1. Classification of the substance or mixture

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

Flammable liquids, Category 2 H225
Skin corrosion/irritation, Category 2 H315
Specific target organ toxicity – Single
exposure, Category 3, Narcosis H336
Aspiration hazard, Category 1 H304
Hazardous to the aquatic environment –
Acute Hazard, Category 1 H400

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

Adverse physicochemical, human health and environmental effects

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Product Code : 42900

Page 2 of 14

Highly flammable liquid and vapour. May cause drowsiness or dizziness. Causes skin irritation. May be fatal if swallowed and enters airways. Very toxic to aquatic life with long lasting effects.

2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]
Hazard pictograms (CLP)



GHS02 GHS07 GHS09

Signal word (CLP)

: Danger

Hazard statements (CLP)

: H225 - Highly flammable liquid and vapour.
H304 - May be fatal if swallowed and enters airways.
H315 - Causes skin irritation.

Precautionary statements (CLP)

: P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
P261 - Avoid breathing dust/fume/gas/mist/vapours/spray.
P273 - Avoid release to the environment.
P303+P361+P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water
P304+P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing.

2.3. Other hazards

Contains no PBT/vPvB substances $\geq 0.1\%$ assessed in accordance with REACH Annex XIII

3. Composition/information on ingredients

3.1. Substances

Name : 2,2,4-TRIMETHYLPENTANE FOR HPLC

CAS-No : 540-84-1

3.2. Mixtures

Not applicable

4. First aid measures

4.1. Description of first aid measures

First-aid measures general : Call a physician immediately.

First-aid measures after inhalation : Remove person to fresh air and keep comfortable for

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Product Code : 42900

Page 3 of 14

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

First-aid measures after skin contact : Wash with plenty of water/.... Wash contaminated clothing before reuse. Get medical advice/attention. Rinse skin with water/shower. Take off immediately all contaminated clothing. If skin irritation occurs: Get medical advice/attention.

First-aid measures after eye contact : Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical advice/attention.

First-aid measures after ingestion : Immediately call a POISON CENTER/doctor. Rinse mouth. Do not induce vomiting. Call a physician immediately.

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

Symptoms/effects after inhalation : May cause drowsiness or dizziness.

Symptoms/effects after skin contact : Causes skin irritation. Irritation

Symptoms/effects after eye contact : None under normal conditions.

Symptoms/effects after ingestion : May be fatal if swallowed and enters airways. Risk of lung oedema.

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

Treat symptomatically.

5. Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Carbon dioxide. Dry powder. Foam. Water spray

Unsuitable extinguishing media : Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

Hazardous decomposition products in case of fire : Toxic fumes may be released.

5.3. Advice for firefighters

Protection during firefighting : Do not attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing.

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Page 4 of 14

6. Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Remove ignition sources. Use special care to avoid static electric charges. No open flames. No smoking. Stop leak if safe to do so. Notify authorities if product enters sewers or public waters. Absorb spillage to prevent material damage.

6.1.1. For non-emergency personnel

Emergency procedures : Ventilate spillage area. Evacuate unnecessary personnel. No open flames, no sparks, and no smoking. Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid contact with skin and eyes.

6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. Use personal protective equipment as required. For further information refer to section 8: "Exposure controls/ personal protection"

Emergency procedures : Ventilate area. Evacuate unnecessary personnel. Stop leak if safe to do so

6.2. Environmental precautions

Avoid release to the environment. Very toxic to aquatic life with long lasting effects.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : Take up liquid spill into absorbent material. On land, sweep or shovel into suitable containers. Collect spillage. Notify authorities if product enters sewers or public waters.

Other information : Dispose of materials or solid residues at an authorized site.

6.4. Reference to other sections

For further information refer to section 13.

7. Handling and storage

7.1. Precautions for safe handling

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EFFECTIVE DATE : 16/06/2025

Product Code : 42900

Page 5 of 14

Precautions for safe handling

: Keep away from sources of ignition - No smoking. Use only non-sparking tools. Avoid contact with skin and eyes. Use only outdoors or in a well-ventilated area. Do not breathe vapours. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Ground/bond container and receiving equipment. Take precautionary measures against static discharge. Flammable vapours may accumulate in the container. Use explosion-proof equipment. Wear personal protective equipment. Avoid breathing dust/fume/gas/mist/vapours/spray.

Hygiene measures

: Wash hands, forearms and face thoroughly after handling. Wash contaminated clothing before reuse. Do not eat, drink or smoke when using this product. Always wash hands after handling the product

7.2. Conditions for safe storage, including any incompatibilities

Technical measures

: Proper grounding procedures to avoid static electricity should be followed. Ground/bond container and receiving equipment.

Storage conditions

: Keep in fireproof place. Keep container tightly closed. Store in a well-ventilated place. Keep cool. Store locked up.

Storage away from

: Open flame. Heat. Sparks. Avoid contact with hot surfaces. No flames, no sparks. Eliminate all sources of ignition.

7.3. Specific end use(s)

No additional information available

8. Exposure controls/personal protection

8.1. Control parameters

8.1.1. National occupational exposure and biological limit values

No additional information available

8.1.2. Recommended monitoring procedures

No additional information available

8.1.3. Air contaminants formed

No additional information available

8.1.4. DNEL and PNEC

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Page 6 of 14

No additional information available

8.1.5. Control banding

No additional information available

8.2. Exposure controls

8.2.1. Appropriate engineering controls

Ensure good ventilation of the work station.

8.2.2. Personal protection equipment

Eye protection : Chemical goggles or safety glasses
Hand protection : Wear protective gloves
Skin protection : Wear suitable protective clothing
Respiratory protection : Wear appropriate mask.
Thermal hazards : No additional information available

8.2.3. Environmental exposure controls

Avoid release to the environment

9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state : Liquid
Appearance : clear liquid
Molecular mass : 114.23 g/mol
Colour : colourless
Odour : characteristic odour
Odour threshold : Not available
pH : Not available
Melting point : Not applicable
Freezing point : -107 °C
Boiling point : 98 – 99 °C
Flash point : -12 °C
Auto-ignition temperature : 418 °C
Decomposition temperature : Not available
Flammability (solid, gas) : Flammable Highly flammable liquid and vapour.
Vapour pressure : 5.1 kPa at 20 °C
Relative vapour density at 20 °C : 3.93 (Air = 1)
Relative density : 0.69
Density : 0.691-0.693g
Solubility : Water: Immiscible

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Product Code : 42900

Page 7 of 14

Partition coefficient n-octanol/water (Log Pow) : 4.6
Viscosity, kinematic : 0.737 mm²/s
Viscosity, dynamic : 0.51 mPa·s at 22 °C

9.2. Other information

Refractive index (n)²⁰_D : 1.391-1.392

10. Stability and reactivity

10.1. Reactivity

Highly flammable liquid and vapour.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

Open flame. Direct sunlight. Avoid contact with hot surfaces. Heat. No flames, no sparks. Eliminate all sources of ignition.

10.5. Incompatible materials

No additional information available

10.6. Hazardous decomposition products

May release flammable gases.

11. Toxicological information

11.1. Information on toxicological effects

Acute toxicity (oral) : Not classified
Acute toxicity (dermal) : Not classified
Acute toxicity (inhalation) : Not classified
Skin corrosion/irritation : Causes skin irritation.
Additional information : Not classified
Serious eye damage/irritation : Not classified
Respiratory or skin sensitisation : Not classified
Germ cell mutagenicity : Not classified
Carcinogenicity : Not classified
Reproductive toxicity : Not classified
STOT-single exposure : May cause drowsiness or dizziness.
STOT-repeated exposure : Not classified

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REVISION DATE : 14/06/2025
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Page 8 of 14

Aspiration hazard : May be fatal if swallowed and enters airways

12. Ecological information

12.1. Toxicity

Ecology - general Very toxic to aquatic life with long lasting effects.
Hazardous to the aquatic environment, Very toxic to aquatic life.
short-term (acute)
Hazardous to the aquatic environment, long- Very toxic to aquatic life with long lasting effects
term (chronic)

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

No additional information available

12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

No additional information available

13. Disposal considerations

13.1. Waste treatment methods

Waste treatment methods : Dispose of contents/container in accordance with licensed collector's sorting instructions
Product/Packaging disposal recommendations : Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation. Disposal must be done according to official regulations.
Additional information : Handle empty containers with care because residual vapours are flammable. Flammable vapours may accumulate in the container. Do not re-use empty containers.

14. Transport information

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Product Code : 42900

Page 9 of 14

In accordance with ADR / IMDG / IATA / ADN / RID

14.1. UN number

UN-No. (ADR) : UN 1262
UN-No. (IMDG) : UN 1262
UN-No. (IATA) : UN 1262
UN-No. (ADN) : UN 1262
UN-No. (RID) : UN 1262

14.2. UN proper shipping name

Proper Shipping Name (ADR) : OCTANES
Proper Shipping Name (IMDG) : OCTANES
Proper Shipping Name (IATA) : Octanes
Proper Shipping Name (ADN) : OCTANES
Proper Shipping Name (RID) : OCTANES
Transport document description (ADR) : UN 1262 OCTANES, 3, II, (D/E)
Transport document description (IMDG) : UN 1262 OCTANES, 3, II, MARINE
POLLUTANT/ENVIRONMENTALLY HAZARDOUS
Transport document description (IATA) : UN 1262 Octanes, 3, II, ENVIRONMENTALLY
HAZARDOUS
Transport document description (ADN) : UN 1262 Octanes, 3, II, ENVIRONMENTALLY
HAZARDOUS
Transport document description (RID) : UN 1262 Octanes, 3, II, ENVIRONMENTALLY
HAZARDOUS

14.3. Transport hazard class(es)

ADR

Transport hazard class(es) (ADR) : 3
Danger labels (ADR) : 3

IMDG

Transport hazard class(es) (IMDG) : 3
Danger labels (IMDG) : 3

IATA

Transport hazard class(es) (IATA) : 3
Danger labels (IATA) : 3

ADN

Transport hazard class(es) (ADN) : 3
Danger labels (ADN) : 3

RID

Transport hazard class(es) (RID) : 3
Danger labels (RID) : 3

14.4. Packing group

Packing group (ADR) : II

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REVISION DATE : 14/06/2025
EFFECTIVE DATE : 16/06/2025

Product Code : 42900

Page 10 of 14

Packing group (IMDG) : II
Packing group (IATA) : II
Packing group (ADN) : II
Packing group (RID) : II

14.5. Environmental hazards

Dangerous for the environment : Yes
Marine pollutant : Yes
Other information : No supplementary information available

14.6. Special precautions for user

Overland transport

Classification code (ADR) : F1
Limited quantities (ADR) : 11
Excepted quantities (ADR) : E2
Packing instructions (ADR) : P001, IBC02, R001
Mixed packing provisions (ADR) : MP19
Portable tank and bulk container instructions (ADR) : T4
Portable tank and bulk container special provisions (ADR) : TP1
Tank code (ADR) : LGBF
Vehicle for tank carriage : FL
Transport category (ADR) : 2
Special provisions for carriage - Operation (ADR) : S2, S20
Hazard identification number (Kemler No.) : 33
Tunnel restriction code (ADR) : D/E
EAC code : 3YE

Transport by sea

Limited quantities (IMDG) : 1 L
Excepted quantities (IMDG) : E2
Packing instructions (IMDG) : P001
IBC packing instructions (IMDG) : IBC02
Tank instructions (IMDG) : T4
Tank special provisions (IMDG) : TP2
EmS-No. (Fire) : F-E
EmS-No. (Spillage) : S-E
Stowage category (IMDG) : B
MFAG-No : 128

Air transport

PCA Excepted quantities (IATA) : E2

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Product Code : 42900

Page 11 of 14

PCA Limited quantities (IATA)	: Y341
PCA limited quantity max net quantity (IATA)	: 1L
PCA packing instructions (IATA)	: 353
PCA max net quantity (IATA)	: 5L
CAO packing instructions (IATA)	: 364
CAO max net quantity (IATA)	: 60L
ERG code (IATA)	: 3H
Inland waterway transport	
Classification code (ADN)	: F1
Limited quantities (ADN)	: 1 L
Excepted quantities (ADN)	: E2
Carriage permitted (ADN)	: T
Equipment required (ADN)	: PP, EX, A
Ventilation (ADN)	: VE01
Number of blue cones/lights (ADN)	: 1
Rail transport	
Classification code (RID)	: F1
Limited quantities (RID)	: 1L
Excepted quantities (RID)	: E2
Packing instructions (RID)	: P001, IBC02, R001
Mixed packing provisions (RID)	: MP19
Portable tank and bulk container instructions (RID)	: T4
Portable tank and bulk container special provisions (RID)	: TP1
Tank codes for RID tanks (RID)	: LGBF
Transport category (RID)	: 2
Colis express (express parcels) (RID)	: CE7
Hazard identification number (RID)	: 33

14.7. Transport in bulk according to Annex II of Marpol and the IBC Code
Not applicable

15. Regulatory information

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

15.1.1 EU-Regulations

EU restriction list (REACH Annex XVII)

Reference code Applicable on

Reference code Applicable on

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EFFECTIVE DATE : 16/06/2025

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Page 12 of 14

3(a)	2,2,4-TRIMETHYLPENTANE
3(b)	2,2,4-TRIMETHYLPENTANE
3(c)	2,2,4-TRIMETHYLPENTANE
40	2,2,4-TRIMETHYLPENTANE

Not listed on REACH Annex XIV (Authorisation List)

Not listed on the REACH Candidate List

Not listed on the PIC list (Regulation EU 649/2012)

Not listed on the POP list (Regulation EU 2019/1021)

Not listed on the Ozone Depletion list (Regulation EU 1005/2009)

Contains no substance subject to the COUNCIL REGULATION (EC) No 428/2009 of 5 May 2009 setting up a Community regime for the control of exports, transfer, brokering and transit of dual-use items.

Contains no substance(s) listed on the Drug Precursors list (Regulation EC 273/2004 on the manufacture and the placing on market of certain substances used in the illicit manufacture of narcotic drugs and psychotropic substances)

15.1.2. National regulations

France

Occupational diseases

Code	Description
RG 84	Conditions caused by liquid organic solvents for professional use: saturated or unsaturated aliphatic or cyclic liquid hydrocarbons and mixtures thereof; liquid halogenated hydrocarbons; nitrated derivatives of aliphatic hydrocarbons; alcohols; glycols, glycol ethers; ketones; aldehydes; aliphatic and cyclic ethers, including tetrahydrofuran; esters; dimethylformamide and dimethylacetamine; acetonitrile and propionitrile; pyridine; dimethylsulfone and dimethylsulfoxide

Germany

Water hazard class (WGK)

: WGK 2, Significantly hazardous to water (Classification according to AwSV; ID No. 479).

Hazardous Incident Ordinance (12. BImSchV)

: Is not subject of the Hazardous Incident Ordinance (12. BImSchV)

Netherlands

SZW-lijst van kankerverwekkende stoffen

: The substance is not listed

SZW-lijst van mutagene stoffen

: The substance is not listed

SZW-lijst van reprotoxische stoffen – Borstvoeding

: The substance is not listed

SZW-lijst van reprotoxische stoffen –

: The substance is not listed

Vruchtbaarheid

SZW-lijst van reprotoxische stoffen –

: The substance is not listed

Ontwikkeling

Denmark

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Material Safety Data Sheet



2,2,4-TRIMETHYLPENTANE FOR HPLC
(iso-Octane)

VERSION : 05
REVISION DATE : 14/06/2025
EFFECTIVE DATE : 16/06/2025

Product Code : 42900

Page 13 of 14

Classification remarks : Emergency management guidelines for the storage of flammable liquids must be followed
Danish National Regulations : Young people below the age of 18 years are not allowed to use the product

15.2. Chemical safety assessment

No chemical safety assessment has been carried out

16. Other information

Abbreviations and acronyms	
ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
ATE	Acute Toxicity Estimate
BCF	Bioconcentration factor
BLV	Biological limit value
BOD	Biochemical oxygen demand
COD	Chemical oxygen demand
COD	Chemical oxygen demand
DMEL	Derived Minimal Effect level
DNEL	Derived-No Effect Level
EC-No.	European Community number
EC50	Median effective concentration
EN	European Standard
IARC	International Agency for Research on Cancer
IATA	International Air Transport Association
IMDG	International Maritime Dangerous Goods
LC50	Median lethal concentration
LD50	Median lethal dose
LOAEL	Lowest Observed Adverse Effect Level
NOAEC	No-Observed Adverse Effect Concentration
NOAEL	No-Observed Adverse Effect Level
NOEC	No-Observed Effect Concentration
OECD	Organisation for Economic Co-operation and Development
OEL	Occupational Exposure Limit
PBT	Persistent Bioaccumulative Toxic

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Page 14 of 14

PNEC	Predicted No-Effect Concentration
RID	Regulations concerning the International Carriage of Dangerous Goods by Rail
SDS	Safety Data Sheet
STP	Sewage treatment plant
ThOD	Theoretical oxygen demand (ThOD)
TLM	Median Tolerance Limit
VOC	Volatile Organic Compounds
CAS-No.	Chemical Abstract Service number
N.O.S.	Not Otherwise Specified
vPvB	Very Persistent and Very Bioaccumulative
ED	Endocrine disrupting properties
Full text of H- and EUH-statements	
Eye Irrit. 2	Serious eye damage/eye irritation, Category 2
Flam. Liq. 2	Flammable liquids, Category 2
STOT SE 3	Specific target organ toxicity — Single exposure, Category 3, Narcosis
H225	Highly flammable liquid and vapour.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.
EUH066	Repeated exposure may cause skin dryness or cracking.

Safety Data Sheet (SDS), EU This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.

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