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

Product name : Isooctane, 2,2,4-trimethylpentane
Type of product : Chemical substance
Product grade : LR, AR/ ACS, HPLC, Certified Dry, GC, Special Grade
CAS No : 540-84-1

1.1. Product Identifiers

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

Identified uses : Reagent for analysis

1.3. Details of the supplier of the safety data sheet

RYZE CHEMIE PRIVATE LIMITED
Gami Industrial Park, Unit.13, Second Floor, C Block,
Plot No.C-39-A, TTC Industrial area, Navi Mumbai,
Thane, Maharashtra-400705
Safety@ryzechemie.com

1.4. Emergency Telephone Number : +91- 9930060404

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Flammable liquids, Category 2	H225: Highly flammable liquid and vapour.
Skin irritation, Category 2	H315: Causes skin irritation.
Specific target organ toxicity - single exposure, Category 3, Central nervous system	H336: May cause drowsiness or dizziness.
Aspiration hazard, Category 1	H304: May be fatal if swallowed and enters airways.

Short-term (acute) aquatic hazard, Category 1	H400: Very toxic to aquatic life.
Long-term (chronic) aquatic hazard, Category 1	H410: Very toxic to aquatic life with long lasting effects.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms :



Signal word : Danger

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 :

Prevention:

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233	Keep container tightly closed.
P273	Avoid release to the environment.

Response:

P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P331	Do NOT induce vomiting.

Reduced Labelling (<= 125 ml)

Hazard pictograms :



Signal word

Hazard Statements

H304 May be fatal if swallowed and enters airways.

Precautionary Statements	
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P331	Do NOT induce vomiting.
Supplemental Hazard Statements	none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1 Substances

Index-No. : 601-009-00-8

EC-No. : 208-759-1

Components

Chemical name	CAS-No. EC-No.	Concentration (% w/w)	M-Factor, SCL, ATE
isooctane	540-84-1 208-759-1	>= 90 - <= 100	M-Factor (Acute aquatic toxicity): 1 M-Factor (Chronic aquatic toxicity): 1 --- specific concentration limit STOT SE 3; H336 >= 20 %

SECTION 4: First aid measures

4.1 Description of first aid measures

General advice : Show this 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	:	After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

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 (CO_2) 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

Specific hazards during fire fighting	:	Combustible. Pay attention to flashback. Vapours 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.
Hazardous combustion products	:	Carbon oxides

5.3 Advice for firefighters

Special protective equipment for fire-fighters	:	Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.
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

Personal precautions : Advice for non-emergency personnel:
Do not breathe vapours, 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

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

6.3 Methods and material for containment and cleaning up

Methods for 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 considerations 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

Further information on storage conditions : Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Storage class (TRGS 510) : 3, Flammable liquids

Further information on storage stability : Recommended storage temperature see product label.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure Limits

Predicted No Effect Concentration (PNEC) according to Regulation (EC) No. 1907/2006

Substance name	Environmental Compartment	Value
	Not applicable	

8.2 Exposure controls

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

Hand protection

Material	:	Nitrile rubber
Break through time	:	480 min
Glove thickness	:	0,4 mm
Protective index	:	Full contact
Manufacturer	:	Camatril® (KCL 730 / Size M)

Material	:	Chloroprene
Break through time	:	120 min
Glove thickness	:	0,65 mm
Protective index	:	Splash contact
Manufacturer	:	KCL 720 Camapren®

Remarks : 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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Skin and 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.

Recommended Filter type:	:	Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Advice	:	Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	:	liquid (20 °C, 1.013 hPa)
Color	:	colourless
Odor	:	No data available
Melting point/ range	:	-107 °C
Boiling point/boiling range	:	99,2 °C (1.000 hPa)
Flammability	:	No data available
Upper explosion limit / Upper flammability limit	:	Upper explosion limit 6 %(V)
Lower explosion limit / Lower flammability limit	:	Lower explosion limit 1 %(V)
Flash point	:	-12 °C Method: closed cup
Autoignition temperature	:	396 °C
Decomposition temperature	:	No data available
pH	:	No data available
Viscosity, dynamic	:	No data available
Viscosity, kinematic	:	No data available
Flow time	:	No data available

Solubility(ies)		
Water solubility	:	insoluble
Partition coefficient: n-octanol/water	:	log Pow: 4,6 Bioaccumulation is not expected.
Vapor pressure	:	55 hPa (21 °C)
		120 hPa (37,80 °C)
Relative density	:	No data available
Density	:	0,69 g/cm3 (15 °C)
Relative vapour density	:	3,94 (Air = 1.0)

9.2 Other information

Explosives	:	Not classified as explosive.
Oxidizing properties	:	none
Burning rate	:	No data available
Evaporation rate	:	No data available
Molecular weight	:	114,23 g/mol

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapours 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

Hazardous reactions	:	Violent reactions possible with: Strong oxidizing agents

10.4 Conditions to avoid

Conditions to avoid : Warming.

10.5 Incompatible materials

Materials to avoid : 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 - vapour

(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
Maximisation 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
No data available

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 oedema and pneumonitis.

11.2 Additional Information

Endocrine disrupting properties

Product:

Assessment	The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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

SECTION 12: Ecological information

12.1 Toxicity

Components:

isooctane:

Toxicity to fish	: LC50 (Oncorhynchus mykiss (rainbow trout)): 0,11 mg/l End point: mortality Exposure time: 96 h Test Type: semi-static test Analytical monitoring: yes Method: OECD Test Guideline 203 GLP: yes

Toxicity to daphnia and other aquatic invertebrates	:	EC50 (Daphnia magna (Water flea)): 0,4 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Remarks: (in analogy to similar products) (ECHA) The value is given in analogy to the following substances: 2,3,4-Trimethylpentane
M-Factor (Acute aquatic toxicity)	:	1
Toxicity to microorganisms	:	EC0 (Pseudomonas putida): 10.000 mg/l Remarks: (IUCLID)
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	:	EC50: 0,23 mg/l Exposure time: 21 d Species: Daphnia magna (Water flea) Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 211 GLP: yes
M-Factor (Chronic aquatic toxicity)	:	1

12.2 Persistence and degradability

Components:

isooctane:

Biodegradability	:	Test Type: aerobic Inoculum: activated sludge Concentration: 49 mg/l Result: Inherently biodegradable. Biodegradation: 51,3 % Exposure time: 28 d Method: OECD Test Guideline 301F

12.3 Bioaccumulative potential

Components:

isooctane:

Bioaccumulation	:	Bioconcentration factor (BCF): 231
Partition coefficient n-octanol/water	:	log Pow: 4,6 Remarks: Bioaccumulation is not expected.

12.4 Mobility in soil

No data available

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12.5 Results of PBT and vPvB assessment

Product:

Assessment : This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Components:

isooctane:

Assessment : Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

12.6 Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

No data available

12.7 Other adverse effects

Components:

isooctane:

Additional ecological information : 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.

SECTION 14: Transport information

14.1 UN number or ID number

ADR	:	UN 1262
IMDG	:	UN 1262
IATA	:	UN 1262

14.2 UN proper shipping name

ADR	:	OCTANES
IMDG	:	OCTANES
IATA	:	Octanes

14.3 Transport hazard class(es)

		Class	Subsidiary risks
ADR	:	3	
IMDG	:	3	
IATA	:	3	

14.4 Packing group

ADR

Packing group	:	II
Classification Code	:	F1
Hazard Identification Number	:	33
Labels	:	3
Tunnel restriction code	:	(D/E)

IMDG

Packing group	:	II
Labels	:	3
EmS Code	:	F-E, S-E

IATA (Cargo)

Packing instruction (cargo aircraft)	:	364
Packing instruction (LQ)	:	Y341
Packing group	:	II
Labels	:	Class 3 - Flammable liquids

IATA_P (Passenger)

Packing instruction (passenger aircraft)	:	353
Packing instruction (LQ)	:	Y341

Packing group : II

Labels : Class 3 - Flammable liquids

14.5 Environmental hazards

ADR

Environmentally hazardous	:	yes

IMDG

Marine pollutant	:	yes

14.6 Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

14.7 Maritime transport in bulk according to IMO instruments

Not applicable for product as supplied.

SECTION 15: Regulatory information

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

REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII)	:	Conditions of restriction for the following entries should be considered: Number on list 3 Number on list 40 Number on list 75: If you intend to use this product as tattoo ink, please contact your vendor.
REACH - Candidate List of Substances of Very High Concern for Authorisation (Article 59).	:	Not applicable
Regulation (EU) No 2024/590 on substances that deplete the ozone layer	:	Not applicable
Regulation (EU) 2019/1021 on persistent organic pollutants (recast)	:	Not applicable
REACH - List of substances subject to authorisation (Annex XIV)	:	Not applicable

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.	P5c	FLAMMABLE LIQUIDS
	E1	ENVIRONMENTAL HAZARDS

15.2 Chemical safety assessment

A Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Abbreviation and Acronyms

CAS - Chemical Abstracts Service
TSCA - United States Toxic Substances Control Act Section 8(b)Inventory
EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances
DSL/NDSL - Canadian Domestic Substances List/Non- Domestic Substances List
PICCS - Philippines Inventory of Chemicals and Chemical Substances
ENCS - Japanese Existing and New Chemical Substances
IECSC - Chinese Inventory of Existing Chemical Substances
AICS - Australian Inventory of Chemical Substances
KECL - Korean Existing and Evaluated Chemical Substances
NZIoC - New Zealand Inventory of Chemicals
WEL - Workplace Exposure Limit
TWA - Time Weighted Average
ACGIH - American Conference of Governmental Industrial Hygienists
IARC - International Agency for Research on Cancer
DNEL - Derived No Effect Level
PNEC - Predicted No Effect Concentration
RPE - Respiratory Protective Equipment
LD50 - Lethal Dose 50%
LC50 - Lethal Concentration 50%
EC50 - Effective Concentration 50%
NOEC - No Observed Effect Concentration
POW- Partition coefficient Octanol:Water
PBT - Persistent, Bioaccumulative, Toxic
vPvB - very Persistent, very Bioaccumulative
ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road
ICAO/IATA - International Civil Aviation Organization/International Air Transport Association
IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code
MARPOL - International Convention for the Prevention of Pollution from Ships
OECD - Organization for Economic Co-operation and Development
ATE - Acute Toxicity Estimate
BCF - Bioconcentration factor
VOC - (Volatile Organic Compound)

Disclaimer: The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

Ryze Chemie will not be held liable for any damage resulting from handling or from contact with the above product

End of safety data sheet