



Preparing for the New Era of Laboratories

MATERIAL SAFETY DATA SHEET (MSDS)

According to regulation (EU) no.1907/2006

ISO-OCTANE AR

PRODUCT CODE	: B-3043
CAS No	: 540-84-1
FORMULA	: C_8H_{18}
UN No	: 1262

MATERIAL SAFETY DATA SHEET (SDS/MSDS)

ISO-OCTANE AR



MSDS Number : 195

Date : Aug 23th, 2024

Version : 1.0

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

- 1.1 Product Name** : ISO-OCTANE AR
Synonyms : 2,2,4-Trimethylpentane, Isobutyltrimethylpentane, Isobutyltrimethylmethane, Iso-Octane
CAS No. : 540-84-1
HS Code : 2901 10 00
Chemical Formula : $\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_3$ C_8H_{18} Hill
Molecular Weight : 114.23 g/mol
Product Code : B-3043
Brand : Labotiq
1.2 Manufacturer : Labotiq
Address : Jl.Terapi Raya AD2-Bumi Menteng Asri Bogor, Jawa Barat Indonesia – 16111
Website : www.labotiq.net
Email : labotiq.id@gmail.com
For information : Phone : (+62-251) 839110, 8311662, Fax : (+62-251) 83135710
Emergency number : +6281316894650
1.3 Application : Laboratory chemicals, Manufacture of substances, General Chemical reagent

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

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

Acute aquatic toxicity (Category 1), H400

Chronic aquatic toxicity (Category 1), H410

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

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram



Signal word

Danger

Hazard statement(s)

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 statement(s)

P210

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

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P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/doctor.
P331	Do NOT induce vomiting.
P370 + P378	In case of fire: Use dry powder or dry sand to extinguish.
P403 + P235	Store in a well-ventilated place. Keep cool.
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

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms	: 2,2,4-Trimethylpentane, Isobutyltrimethylpentane, Isobutyltrimethylmethane, Iso-Octane		
Formula	: $\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_3$	C_8H_{18}	Hill
Molecular weight	: 114.23 g/mol		
CAS-No.	: 540-84-1		
EC-No.	: 208-759-1		
Index-No.	: 601-009-00-8		

3.2 Mixture

Hazardous ingredients according to Regulation (EC) No 1272/2008

Component	Classification	Concentration
2,2,4-Trimethylpentane CAS-No. 540-84-1 EC-No. 208-759-1 Index-No. 601-009-00-8	Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H315, H336, H304, H400, H410 M-Factor - Aquatic Acute: 10	<=100 %

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

Consult a physician. Show this safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

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If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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 Combustible. Pay attention to flashback. Vapors are heavier than air and may spread along floors. Risk of dust explosion. 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. Chemisorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

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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****8.2 Exposure controls****Appropriate engineering controls**

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

Personal protective equipment**Eye/face protection**

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin 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.

The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740, Size M)

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Splash contact

Material: Nitrile rubber
 Minimum layer thickness: 0.11 mm
 Break through time: 480 min
 Material tested: Dermatrill® (KCL 740, Size M)

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use (EN 143) respirator cartridges as a backup to engineering controls. If the full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance	Form: liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: -107 °C
Initial boiling point and boiling range	98 - 99 °C
Flash point	-12 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 6 %(V) Lower explosion limit: 1 %(V)
Vapour pressure	No data available
	55 hPa at 21 °C
	120 hPa at 37,80 °C
Vapour density	3,94 - (Air = 1.0)
Relative density	0,692 g/mL at 25 °C
Water solubility	No data available
Partition coefficient: n-octanol/water	log Pow: 4,6 - Bioaccumulation is not expected.
Auto-ignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

9.2 Other safety information

Relative vapor density	3,94 - (Air = 1.0)
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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

Hazardous decomposition products formed under fire conditions. - Carbon oxides
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 (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)

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 sensitisation

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

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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 component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available(2,2,4-Trimethylpentane)

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness. - Central nervous system

Specific target organ toxicity - repeated exposure

No data available(2,2,4-Trimethylpentane)

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

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

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)

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

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12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB 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.

12.6 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

Burn in a chemical incinerator equipped with an afterburner and scrubber b highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1262

IMDG: 1262

IATA: 1262

14.2 UN proper shipping name

ADR/RID: OCTANES

IMDG: OCTANES

IATA: OCTANES

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA: 3

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA: II

14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA: no

14.6 Special precautions for user

Further information

No data available

SECTION 15: Regulatory information

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

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

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Full text of H-Statements referred to under sections 2 and 3.

- 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.
- H400 Very toxic to aquatic life.
- H410 Very toxic to aquatic life with long lasting effects.

National Fire Protection Association (U.S.A.):

Health: 1

Flammability: 3

Reactivity: 0

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. Labotiq shall not be held liable for any damage resulting from handling or from contact with the above product.

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