

Safety Data Sheet

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifier**

Trade name/designation:	iso-Octane AR, ACS
Product No.:	O0019
Synonymes:	2,2,4-Trimethylpentane
CAS No.	540-84-1

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

Relevant identified uses:	General chemical reagent
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1.3 Details of the supplier of the safety data sheet**Supplier****Avantor Performance Materials India Ltd.**

Street	501, 5th floor, Tiffany Building, Hiranandani Business Park,
Postal code/city	Thane, Maharashtra - 400607, India
Telephone	022-41288100

Emergency phone number

Telephone	1800105561
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Preparation Information

Product Information Compliance

1.4 E-mail

SDS@avantorsciences.com

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Physical hazards

Flammable liquid, category 2

health hazards

Aspiration hazard, category 1

Skin irritation, category 2

Specific target organ toxicity (single exposure), category 3, narcotic effect

Environmental hazards

Hazardous to the aquatic environment, chronic, category 1

2.2 Label elements

Hazard pictograms



Signal word: Danger

Highly flammable liquid and vapour.

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.

2.3 Other hazards none

SECTION 3: Composition / information on ingredients

Substances

Substance name	2,2,4-Trimethylpentane
Molecular formula	$(\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{CH}_3)_3$
Molecular weight	114.23 g/mol
CAS No.	540-84-1

SECTION 4: First aid measures

4.1 General information

IF exposed: Immediately call a POISON CENTRE/doctor. If unconscious place in recovery position and seek medical advice. Never give anything by mouth to an unconscious person or a person with cramps. Change contaminated, saturated clothing. Do not leave affected person unattended.

After inhalation

Immediately call a POISON CENTRE/doctor. Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

In case of skin contact

After contact with skin, wash immediately with plenty of water and soap. Remove contaminated, saturated clothing immediately. In case of skin reactions, consult a physician.

After eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist. Protect uninjured eye. Remove contact lenses, if present and easy to do. Continue rinsing.

In case of ingestion

Immediately call a POISON CENTRE/doctor. Do NOT induce vomiting. Rinse mouth thoroughly with water. Give nothing to eat or drink.

4.2 Most important symptoms and effects, both acute and delayed

no data available

4.3 Indication of any immediate medical attention and special treatment needed

no data available

no data available

SECTION 5: Firefighting measures

5.1 Extinguishing media**Suitable extinguishing media**

Water spray
ABC-powder
Carbon dioxide (CO₂)
Nitrogen

Extinguishing media which must not be used for safety reasons

no restriction

5.2 Special hazards arising from the substance or mixture

In case of fire may be liberated:
Carbon monoxide
Carbon dioxide (CO₂)

5.3 Advice for firefighters

DO NOT fight fire when fire reaches explosives.
Special protective equipment for firefighters
Wear a self-contained breathing apparatus and chemical protective clothing.

5.4 Additional information

Do not allow run-off from fire-fighting to enter drains or water courses.
Do not inhale explosion and combustion gases.
Use caution when applying carbon dioxide in confined spaces. Carbon dioxide can displace oxygen.
Use water spray jet to protect personnel and to cool endangered containers.
In case of fire: Evacuate area.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

In case of major fire and large quantities: Remove persons to safety.

6.2 Environmental precautions

Discharge into the environment must be avoided.

6.3 Methods and material for containment and cleaning up

Spilled product must never be returned to the original container for recycling. Collect in closed and suitable containers for disposal.

6.4 Additional information

Clear spills immediately.

SECTION 7: Handling and storage

Precautions for safe handling

Avoid:

Inhalation

Avoid contact with eyes and skin.

Use extractor hood (laboratory).

If handled uncovered, arrangements with local exhaust ventilation have to be used.

If local exhaust ventilation is not possible or not sufficient, the entire working area must be ventilated by technical means.

Keep away from sources of ignition - No smoking.

Usual measures for fire prevention.

Take precautionary measures against static discharges.

Conditions for safe storage, including any incompatibilities

Recommended storage temperature: Keep bottles tightly closed and away from sources of ignition and heat.

Keep container tightly closed and in a well-ventilated place. Keep/Store away from combustible materials.

Specific end use(s)

no data available

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Does not contain substances above concentration limits fixing an occupational exposure limit.

8.2 Exposure controls

Appropriate engineering controls

no data available

Personal protection equipment

no data available

Eye/face protection

no data available

Skin protection

Wear suitable gloves. When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. In the case of wanting to use the gloves again, clean them before taking off and air them well. Check leak tightness/impermeability prior to use.

By short-term hand contact

Suitable material:	NBR (Nitrile rubber)
Thickness of the glove material:	0,12 mm
Breakthrough time (maximum wearing time):	> 480 min

By long-term hand contact

Suitable material:	NBR (Nitrile rubber)
Thickness of the glove material:	0,38 mm
Breakthrough time (maximum wearing time):	> 480 min

Respiratory protection

no data available

Additional information

no data available

Environmental exposure controls

no data available

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|----------------------|-------------------|
| (a) Appearance | |
| Physical state: | liquid |
| Colour: | colourless |
| (b) Odour: | no data available |
| (c) Odour threshold: | no data available |

Safety relevant basic data

- | | |
|--|-------------------------------------|
| (d) pH: | 7 (20 °C) |
| (e) Melting point/freezing point: | -107 °C |
| (f) Initial boiling point and boiling range: | 99.2 °C (1013 hPa) |
| (g) Flash point: | -12 °C |
| (h) Evaporation rate: | no data available |
| (i) Flammability (solid, gas): | Highly flammable liquid and vapour. |
| (j) Flammability or explosive limits | |
| Lower explosion limit: | 1 % (v/v) |
| Upper explosion limit: | 6 % (v/v) |
| (k) Vapour pressure: | 41 mmHg (21 °C) |
| (l) Vapour density: | 3.93 (20 °C) |
| (m) Relative density: | 0.692 g/cm ³ (20 °C) |
| (n) Solubility(ies) | |
| Water solubility (g/L): | 560 µg/l (25 °C) |
| Soluble (g/L) in Ethanol: | no data available |
| (o) Partition coefficient: n-octanol/water: | 4.5 (20 °C) |
| (p) Auto-ignition temperature: | 410 °C |
| (q) Decomposition temperature: | no data available |
| (r) Viscosity | |
| Kinematic viscosity: | no data available |
| Dynamic viscosity: | 0.5 mPa*s (20 °C) |
| (s) Explosive properties: | not applicable |
| (t) Oxidising properties: | not applicable |

9.2 Other information

- | | |
|------------------------|-------------------------|
| Bulk density: | no data available |
| Refraction index: | 1.38962 (589 nm; 20 °C) |
| Dissociation constant: | no data available |
| Surface tension: | no data available |
| Henry's Law Constant: | no data available |

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapours can form explosive mixtures with air.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Formation of explosive mixtures with:
Oxidising agent, strong

10.4 Conditions to avoid

This material is combustible and can be ignited by heat, sparks, flames, or other sources of ignition (e.g. static electricity, pilot lights, or mechanical/electrical equipment).

10.5 Incompatible materials

Rubber articles
Plastic articles

10.6 Hazardous decomposition products

no data available

SECTION 11: Toxicological information**11.1 Information on toxicological effects****Acute effects**

Acute oral toxicity:

LD50: < 2500 mg/kg - Rat - (IUCLID)

Acute dermal toxicity:

no data available

Acute inhalation toxicity:

LC50: 47.4 mg/l - Rat - (IUCLID)

Irritant and corrosive effects

Primary irritation to the skin:

Causes skin irritation.

Irritation to eyes:

not applicable

Irritation to respiratory tract:

not applicable

Respiratory or skin sensitisation

In case of skin contact: not sensitising

After inhalation: not sensitising

STOT-single exposure

May cause drowsiness or dizziness.

STOT-repeated exposure

not applicable

CMR effects (carcinogenicity, mutagenicity and toxicity for reproduction)**Carcinogenicity****Germ cell mutagenicity**

No indications of human germ cell mutagenicity exist.

Reproductive toxicity

No indications of human reproductive toxicity exist.

Aspiration hazard

May be fatal if swallowed and enters airways.

Other adverse effects

no data available

SECTION 12: Ecological information

12.1 Ecotoxicity**Fish toxicity:**

no data available

Daphnia toxicity:

no data available

Algae toxicity:

no data available

Bacteria toxicity:

no data available

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water: 4.5 (20 °C)

12.4 Mobility in soil:

no data available

12.5 Results of PBT/vPvB assessment

no data available

12.6 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Appropriate disposal / Product

Dispose according to local legislation. Consult the appropriate local waste disposal expert about waste disposal.

Appropriate disposal / Package

Dispose according to local legislation. Handle contaminated packages in the same way as the substance itself.

SECTION 14: Transport information

Land transport (ADR/RID)

14.1	UN-No.:	1262
14.2	Proper Shipping Name:	OCTANES
14.3	Class(es):	3
	Classification code:	F1
	Hazard label(s):	3
14.4	Packing group:	II
14.5	Environmental hazards:	Dangerous for the environment
14.6	Special precautions for user:	
	Hazard identification number (Kemler No.):	33
	tunnel restriction code:	D/E
		(Passage forbidden through tunnels of category D when carried in bulk or in tanks. Passage forbidden through tunnels of category E.)

Sea transport (IMDG)

14.1	UN-No.:	1262
14.2	Proper Shipping Name:	OCTANES
14.3	Class(es):	3
	Classification code:	
	Hazard label(s):	3
14.4	Packing group:	II
14.5	Environmental hazards:	Dangerous for the environment
	Marine pollutant:	Yes (P)
14.6	Special precautions for user:	
	Segregation group:	-
	EmS-No.	F-E S-E
14.7	Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	
	not relevant	

Air transport (ICAO-TI / IATA-DGR)

14.1	UN-No.:	1262
14.2	Proper Shipping Name:	OCTANES
14.3	Class(es):	3
	Classification code:	
	Hazard label(s):	3
14.4	Packing group:	II
14.5	Special precautions for user:	

SECTION 15: Regulatory information

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

SECTION 16: Other information

Abbreviations and acronyms

ACGIH - American Conference of Governmental Industrial Hygienists
ADR - European Agreement concerning the International Carriage of Dangerous Goods by Road
AGS - Committee on Hazardous Substances (Ausschuss für Gefahrstoffe)
CLP - Regulation on Classification, Labelling and Packaging of Substances and Mixtures
DFG - German Research Foundation (Deutsche Forschungsgemeinschaft)
Gestis - Information system on hazardous substances of the German Social Accident Insurance (Gefahrstoffinformationssystem der Deutschen Gesetzlichen Unfallversicherung)
IATA-DGR - International Air Transport Association-Dangerous Goods Regulations
ICAO-TI - International Civil Aviation Organization-Technical Instructions
IMDG - International Maritime Code for Dangerous Goods
LTV - Long Term Value
NIOSH - National Institute for Occupational Safety and Health
OSHA - Occupational Safety & Health Administration
PBT - Persistent, Bioaccumulative and Toxic
RID - Regulation concerning the International Carriage of Dangerous Goods by Rail
STV - Short Term Value
SVHC - Substances of Very High Concern
vPvB - very Persistent, very Bioaccumulative

Additional information

Indication of changes: general update

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