

SAFETY DATA SHEET

Version 6.4 Revision Date 26.10.2023 Print Date 22.01.2024

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

1.1 Product identifiers

Product name : I - Fenchone

Product Number : W507709
Brand : Aldrich
CAS-No. : 7787-20-4

1.2 Other means of identification

(−)-1,3,3-Trimethyl-2-norbornanone

(1R)-1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one

(1R)-(-)-Fenchone (-)-Fenchone

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

Identified uses : For R&D use only. Not for pharmaceutical, household or other

uses.

1.4 Details of the supplier of the safety data sheet

Company : Merck Life Science Ltd

Level 26 PwC Tower, 15 Customs Street West

1010 AUCKLAND NEW ZEALAND

Telephone : 0800 936 666

E-mail address : customersupport.anz@merckgroup.com

1.5 Emergency telephone

Emergency Phone # : 0800 0800 425 459 (CHEMTREC NZ)

+64 9 801 0034 (Int'l CHEMTREC)

SECTION 2: Hazards identification

2.1 GHS Classification

Flammable liquids (Category 4), H227

Hazardous to the aquatic environment - chronic hazard (Category 2), H411

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

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal Word Warning

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Hazard statement(s)

H227 Combustible liquid.

H411 Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and

other ignition sources. No smoking.

P273 Avoid release to the environment.

Response

P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant

foam to extinguish.

P391 Collect spillage.

Storage

P403 Store in a well-ventilated place.

Disposal

P501 Dispose of contents/ container to an approved waste disposal

plant.

2.3 Other hazards - none

SECTION 3: Composition/information on ingredients

Substance / Mixture : Substance

3.1 Substances

Synonyms : (-)-1,3,3-Trimethyl-2-norbornanone

(1R)-1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one

(1R)-(-)-Fenchone (-)-Fenchone

Hazardous ingredients

Component	Classification	Concentration
(1R)-1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one		
	Flam. Liq. 4; Aquatic Chronic 2; H227, H411	<= 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

If inhaled

After inhalation: fresh air.

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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: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

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

Foam Carbon dioxide (CO2) 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.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

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. 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.

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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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

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

Change contaminated clothing. Wash hands after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

Storage class

Storage class (TRGS 510): 10: Combustible 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

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Wash hands after working with substance.

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

Skin protection

not required

Respiratory protection

Not required; except in case of aerosol formation.

Control of environmental exposure

Do not let product enter drains.

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SECTION 9: Physical and chemical properties

Information on basic physical and chemical properties

Physical state oily

b) Color colorless

c) Odor No data available

d) Melting Melting point/range: 5 - 6 °C - lit.

point/freezing point

e) Initial boiling point 192 - 194 °C - lit. and boiling range

Flammability (solid, f) No data available gas)

g) Upper/lower flammability or

explosive limits

No data available

h) Flash point 66.5 °C - closed cup - Regulation (EC) No. 440/2008, Annex, A.9

i) Autoignition No data available temperature

Decomposition No data available j) temperature

No data available k) pH

Viscosity, kinematic: No data available I) Viscosity Viscosity, dynamic: No data available

1.983 g/l at 20 °C - OECD Test Guideline 105 m) Water solubility log Pow: 2.54 at 20 °C - OECD Test Guideline 107

n) Partition coefficient: n-octanol/water

o) Vapor pressure 306.63 hPa at 25 °C - OECD Test Guideline 104

0.948 g/cm3 at 25 °C - lit. p) Density

No data available Relative density No data available q) Relative vapor density

r) Particle No data available

characteristics

No data available s) Explosive properties

Oxidizing properties

9.2 Other safety information

No data available

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SECTION 10: Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

Strong oxidizing agents

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 - female - > 2,000 mg/kg

(OECD Test Guideline 423)

Remarks: No mortality observed at this dose.

Inhalation: No data available Dermal: No data available

Skin corrosion/irritation

Skin - human skin

Result: No skin irritation (OECD Test Guideline 439)

Serious eye damage/eye irritation

Eyes - Bovine cornea Result: No eye irritation (OECD Test Guideline 437)

Respiratory or skin sensitization

see user defined free text Result: Not a skin sensitizer. (OECD Test Guideline 442C)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

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No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates

static test EC50 - Daphnia magna (Water flea) - 4.373 mg/l - 48 h

(OECD Test Guideline 202)

Toxicity to algae Ecx - Pseudokirchneriella subcapitata (green algae) - 27.35 mg/l -

72 h

(OECD Test Guideline 201)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 61.7 % - Not readily biodegradable.

(OECD Test Guideline 301F)

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available



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

ADR/RID: 3082 IMDG: 3082 IATA-DGR: 3082

14.2 UN proper shipping name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.

((1R)-1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.

((1R)-1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one)

IATA-DGR: Environmentally hazardous substance, liquid, n.o.s. ((1R)-1,3,3-

Trimethylbicyclo[2.2.1]heptan-2-one)

14.3 Transport hazard class(es)

ADR/RID: 9 IMDG: 9 IATA-DGR: 9

14.4 Packaging group

ADR/RID: III IMDG: III IATA-DGR: III

14.5 Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA-DGR: yes

14.6 Special precautions for user

14.7 Incompatible materials

Strong oxidizing agents

Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

Other regulations

Hazchem Code : ●3Z

SECTION 15: Regulatory information

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

National regulatory information

HSNO Approval Code:

HSNO Group Standard Approval: HSR002596 - Laboratory Chemicals and Reagent Kits

Group Standard 2006

Tracking Required: not required Approved Handler Cert.: not required

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SECTION 16: Other information

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

H227 Combustible liquid.

H411 Toxic to aquatic life with long lasting effects.

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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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