

SAFETY DATA SHEET

Version 6.5
Revision Date 03/02/2024
Print Date 07/14/2024**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2-Isopropyl-5-methyl-2-hexenal

Product Number : W340618
Brand : Aldrich
CAS-No. : 35158-25-9**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheetCompany : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATESTelephone : +1 314 771-5765
Fax : +1 800 325-5052**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**Flammable liquids (Category 4), H227
Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319
Skin sensitization (Category 1), H317

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Short-term (acute) aquatic hazard (Category 2), H401

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

Hazard Statements

H227 Combustible liquid.
H315 Causes skin irritation.
H317 May cause an allergic skin reaction.
H319 Causes serious eye irritation.
H401 Toxic to aquatic life.

Precautionary Statements

P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264 Wash skin thoroughly after handling.
P272 Contaminated work clothing must not be allowed out of the workplace.
P273 Avoid release to the environment.
P280 Wear protective gloves/ eye protection/ face protection.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P337 + P313 If eye irritation persists: Get medical advice/ attention.
P362 Take off contaminated clothing and wash before reuse.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235 Store in a well-ventilated place. Keep cool.
P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula : C₁₀H₁₈O
Molecular weight : 154.25 g/mol
CAS-No. : 35158-25-9
EC-No. : 252-406-4

| Component | Classification | Concentration |
|---------------------------------------|------------------------------|---------------|
| 2-Isopropyl-5-methylhex-2-enal | Flam. Liq. 4; Skin Irrit. 2; | <= 100 % |

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| | | |
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| | Eye Irrit. 2A; Skin Sens. 1; Aquatic Acute 2; H227, H315, H319, H317, H401 | |
| DL-α-Tocopherol | | |
| | Skin Sens. 1; H317 | $\geq 0.1 - < 1$ % |

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

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

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.

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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

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.

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

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

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

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face 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

required

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter type ABEK

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.

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.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---------------------------------|----------------------------------|
| a) Appearance | Form: liquid Color: colorless |
| b) Odor | characteristic |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | No data available |
| f) Initial boiling point | 189 °C 372 °F - lit. |

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| | and boiling range | |
| g) | Flash point | 63 °C (145 °F) - closed cup |
| h) | Evaporation rate | No data available |
| i) | Flammability (solid, gas) | No data available |
| j) | Upper/lower flammability or explosive limits | No data available |
| k) | Vapor pressure | No data available |
| l) | Vapor density | No data available |
| m) | Density | 0.845 g/cm ³ at 25 °C (77 °F) - lit. |
| | Relative density | No data available |
| n) | Water solubility | No data available |
| o) | Partition coefficient: n-octanol/water | No data available |
| p) | Autoignition temperature | No data available |
| q) | Decomposition temperature | No data available |
| r) | Viscosity | No data available |
| s) | Explosive properties | No data available |
| t) | Oxidizing properties | No data available |

9.2 Other safety information

No data available

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 - male and female - 6,800 mg/kg

Remarks: (ECHA)

The value is given in analogy to the following substances: citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers)

Inhalation: No data available

LD50 Dermal - Rat - male and female - > 2,000 mg/kg

Remarks: (ECHA)

The value is given in analogy to the following substances: citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers)

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin.

Remarks: (ECHA)

The value is given in analogy to the following substances: citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: positive

(OECD Test Guideline 406)

The value is given in analogy to the following substances: citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers)

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

The value is given in analogy to the following substances: citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers) Test Type: gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

The value is given in analogy to the following substances: citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers) Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

The value is given in analogy to the following substances: citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers)

Test Type: Micronucleus test

Species: Mouse

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

The value is given in analogy to the following substances: citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers)

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

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

Repeated dose toxicity - Rat - male and female - Oral - 104 - 105 Weeks - NOAEL (No observed adverse effect level) - 100 mg/kg - LOAEL (Lowest observed adverse effect level) - 210 mg/kg

The value is given in analogy to the following substances: citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers)

RTECS: MP6450000

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 fish static test LC50 - Leuciscus idus (Golden orfe) - 6.78 mg/l - 96 h (DIN 38412)

Toxicity to daphnia static test EC50 - Daphnia magna (Water flea) - 6.8 mg/l - 48 h

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| and other aquatic invertebrates | Remarks: (ECHA) The value is given in analogy to the following substances: citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers) |
| Toxicity to algae | static test ErC50 - Desmodesmus subspicatus (green algae) - 103.8 mg/l - 72 h Remarks: (ECHA) The value is given in analogy to the following substances: citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers) |
| Toxicity to bacteria | static test EC50 - activated sludge - ca. 160 mg/l - 30 min (OECD Test Guideline 209) |

12.2 Persistence and degradability

No data available

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

DOT (US)

NA-Number: 1993 Class: NONE Packing group: III
Proper shipping name: Combustible liquid, n.o.s. (2-Isopropyl-5-methylhex-2-enal)
Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG

Not dangerous goods

IATA

Not dangerous goods

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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