

SAFETY DATA SHEET

Version 5.11
Revision Date 04/19/2017
Print Date 11/11/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : (±)-Citronellal

Product Number : W230707

Brand : Aldrich

CAS-No. : 106-23-0

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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

Acute toxicity, Oral (Category 4), H302

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

Skin sensitisation (Category 1), H317

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

Acute aquatic toxicity (Category 2), H401

Chronic aquatic toxicity (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

Hazard statement(s)

| | |
|------|--------------------------------------------------|
| H227 | Combustible liquid. |
| H302 | Harmful if swallowed. |
| H315 | Causes skin irritation. |
| H317 | May cause an allergic skin reaction. |
| H319 | Causes serious eye irritation. |
| H335 | May cause respiratory irritation. |
| H411 | Toxic to aquatic life with long lasting effects. |

Precautionary statement(s)

| | |
|--------------------|----------------------------------------------------------------------------------------------------------------------------------|
| P210 | Keep away from heat/sparks/open flames/hot surfaces. No smoking. |
| P261 | Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray. |
| P264 | Wash skin thoroughly after handling. |
| P270 | Do not eat, drink or smoke when using this product. |
| P271 | Use only outdoors or in a well-ventilated area. |
| P272 | Contaminated work clothing should not be allowed out of the workplace. |
| P273 | Avoid release to the environment. |
| P280 | Wear protective gloves/ eye protection/ face protection. |
| P301 + P312 + P330 | IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth. |
| P302 + P352 | IF ON SKIN: Wash with plenty of soap and water. |
| P304 + P340 + P312 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell. |
| 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. |
| P391 | Collect spillage. |
| P403 + P233 | Store in a well-ventilated place. Keep container tightly closed. |
| P403 + P235 | Store in a well-ventilated place. Keep cool. |
| P405 | Store locked up. |
| P501 | Dispose of contents/ container to an approved waste disposal plant. |

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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : (±)-3,7-Dimethyl-6-octenal

Formula : C₁₀H₁₈O

Molecular weight : 154.25 g/mol

CAS-No. : 106-23-0

Hazardous components

| Component | Classification | Concentration |
|----------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|---------------|
| Citronellal | | |
| | Flam. Liq. 4; Skin Irrit. 2; Eye Irrit. 2A; Skin Sens. 1; STOT SE 3; Aquatic Acute 2; Aquatic Chronic 2; H227, H315, H317, H319, H335, H411 | 90 - 100 % |
| Isopulegol | | |
| | Flam. Liq. 4; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H227, H302, H315, H319, H335 | 5 - 10 % |
| 3,7-Dimethyloctanal | | |
| | Flam. Liq. 4; Skin Irrit. 2; Eye Irrit. 2A; H227, H315, H319 | 1 - 5 % |
| Citral | | |
| | Skin Irrit. 2; Skin Sens. 1; Aquatic Acute 2; H315, H317, H401 | 1 - 5 % |

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

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. Move out of dangerous area.

If inhaled

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

In case of skin contact

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.

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

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Unsuitable extinguishing media

Do NOT use water jet.

5.2 Special hazards arising from the substance or mixture

No data available

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.
For personal protection see section 8.

6.2 Environmental precautions

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

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Air and moisture sensitive. Heat sensitive. Handle under inert gas. Protect from moisture.

7.3 Specific end use(s)

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

| Component | CAS-No. | Value | Control parameters | Basis |
|-----------|-----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------|-----------------------------------------|
| Citral | 5392-40-5 | TWA | 5.000000 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Upper Respiratory Tract irritation Eye damage body weight effects Adopted values or notations enclosed are those for which changes are proposed in the NIC See Notice of Intended Changes (NIC) Not classifiable as a human carcinogen Danger of cutaneous absorption Sensitizer | | |
| | | TWA | 5 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | | Dermal Sensitization Upper Respiratory Tract irritation Eye damage body weight effects 2015 Adoption Not classifiable as a human carcinogen Danger of cutaneous absorption | | |

Hazardous components without workplace 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.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 480 min

Material tested:Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.2 mm

Break through time: 30 min

Material tested:Dermatril® P (KCL 743 / Aldrich Z677388, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

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 a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a 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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | |
|-------------------------------------------------|-----------------------------------------------------------------|
| a) Appearance | Form: liquid |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | No data available |
| f) Initial boiling point and boiling range | 207 °C (405 °F) - lit. |
| g) Flash point | 86 °C (187 °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) Vapour pressure | 0.16 hPa (0.12 mmHg) at 20 °C (68 °F) - OECD Test Guideline 104 |
| l) Vapour density | No data available |
| m) Relative density | 0.857 g/mL at 25 °C (77 °F) - lit. |
| n) Water solubility | 0.088 g/l at 25 °C (77 °F) |
| o) Partition coefficient: n-octanol/water | log Pow: 3.62 at 25 °C (77 °F) - OECD Test Guideline 107 |
| p) Auto-ignition temperature | 202 °C (396 °F) at 1,013 hPa (760 mmHg) |
| q) Decomposition temperature | No data available |

- r) Viscosity 1.82 mm²/s at 20 °C (68 °F) -
- s) Explosive properties No data available
- t) Oxidizing properties No data available

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Strong oxidizing agents, Strong acids, Strong bases

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 2,420 mg/kg

Inhalation: No data available

LD50 Dermal - Rabbit - 2,500 - 5,000 mg/kg

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin.

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

reverse mutation assay

S. typhimurium

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.

NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

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

Additional Information

RTECS: Not available

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates static test EC50 - Daphnia magna (Water flea) - 8.7 mg/l - 48 h

Toxicity to algae static test EC50 - Desmodesmus subspicatus (Scenedesmus subspicatus) - 13.33 mg/l - 72 h

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 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Toxic to aquatic life with long lasting effects.

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

NA-Number: 1993 Class: NONE Packing group: III
Proper shipping name: Combustible liquid, n.o.s. (3,7-Dimethyloctanal)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 3082 Class: 9 Packing group: III EMS-No: F-A, S-F
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (3,7-Dimethyloctanal)
Marine pollutant: yes

IATA

UN number: 3082

Class: 9

Packing group: III

Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (3,7-Dimethyloctanal)

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.

15. REGULATORY INFORMATION**SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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.

Pennsylvania Right To Know Components

| | CAS-No. | Revision Date |
|---------------------|-----------|---------------|
| Citronellal | 106-23-0 | |
| Isopulegol | 89-79-2 | |
| 3,7-Dimethyloctanal | 5988-91-0 | |

| | CAS-No. | Revision Date |
|-------------|----------|---------------|
| Citronellal | 106-23-0 | |
| Isopulegol | 89-79-2 | |

New Jersey Right To Know Components

| | CAS-No. | Revision Date |
|---------------------|-----------|---------------|
| Citronellal | 106-23-0 | |
| Isopulegol | 89-79-2 | |
| 3,7-Dimethyloctanal | 5988-91-0 | |
| Citral | 5392-40-5 | |

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION**Full text of H-Statements referred to under sections 2 and 3.**

| | |
|-----------------|--------------------------------------------------|
| Acute Tox. | Acute toxicity |
| Aquatic Acute | Acute aquatic toxicity |
| Aquatic Chronic | Chronic aquatic toxicity |
| Eye Irrit. | Eye irritation |
| Flam. Liq. | Flammable liquids |
| H227 | Combustible liquid. |
| H302 | Harmful if swallowed. |
| H315 | Causes skin irritation. |
| H317 | May cause an allergic skin reaction. |
| H319 | Causes serious eye irritation. |
| H335 | May cause respiratory irritation. |
| H401 | Toxic to aquatic life. |
| H411 | Toxic to aquatic life with long lasting effects. |
| Skin Irrit. | Skin irritation |
| Skin Sens. | Skin sensitisation |

STOT SE Specific target organ toxicity - single exposure

HMIS Rating

| | |
|------------------------|---|
| Health hazard: | 2 |
| Chronic Health Hazard: | |
| Flammability: | 2 |
| Physical Hazard | 0 |

NFPA Rating

| | |
|--------------------|---|
| Health hazard: | 2 |
| Fire Hazard: | 2 |
| Reactivity Hazard: | 0 |

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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