Citral SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Citral
* Catalog Number: S5138
* CAS Number: 5392-40-5
* IUPAC Name: 2,6-Octadienal, 3,7-dimethyl-

Relevant identified uses and uses advised against

* Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.
* Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

* Company: Selleck Chemicals
* TollFree: +1 877 796-6397
* Tel: +1 832 582-8158
* Fax: +1 832 582-8590

Emergency telephone number

* Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

Flammable liquids: Category 4. H227
Skin irritation: Category 2. H315
Skin sensitization: Category 1. H317
Serious eye irritation: Category 2. H319
Reproductive toxicity: Category 2. H361

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)	
Signal Word	Warning
Hazard statement(s)	H227: Combustible liquid H315: Causes skin irritation H317: May cause an allergic skin reaction H319: Causes serious eye irritation H361: Suspected of damaging fertility or the unborn child
Precautionary statement(s)	None.

Prevention	P203: Obtain, read and follow all safety instructions before use. P210: Keep away from heat, hot surface, sparks, open flames and other ignition sources. No smoking. P261: Avoid breathing dust/fume/gas/mist/vapors/spray. P264: Wash hands thoroughly after handling. P264+P265: Wash hands thoroughly after handling. Do not touch eyes. P272: Contaminated work clothing should not be allowed out of the workplace. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
Response	P302+P352: IF ON SKIN: wash with plenty of water. P305+P351: IF IN EYES: Rinse cautiously with water for several minutes. P318: if exposed or concerned, get medical advice. P321: Specific treatment (see information on this label and safety datasheet)). P332+P317: If skin irritation occurs: Get medical help. P333+P317: If skin irritation or rash occurs: Get medical help. P337+P317: If eye irritation persists: Get medical help. P338: Remove contact lenses, if present and easy to do. Continue rinsing. P362+P364: Take off contaminated clothing and wash it before reuse. P370+P378: In case of fire: Use water spray, dry chemical, carbon dioxide, or appropriate foam to extinguish.
Storage	P403: Store in a well-ventilated place. P405: Store locked up.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: Citral

CAS Number: 5392-40-5

PubChem CID: 638011

Molecular formula: C10H16O

Molecular weight: 152.23 g/mol

IUPAC name: (2E)-3,7-dimethylocta-2,6-dienal

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Fresh air, rest.

Skin contact: Rinse and then wash skin with water and soap.

Eye contact: Rinse with plenty of water (remove contact lenses if easily possible).

Ingestion: Rinse mouth.

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO2), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

SMALL FIRE: Dry chemical, CO2 or water spray.

LARGE FIRE: Dry chemical, CO2, alcohol-resistant foam or water spray. If it can be done safely, move undamaged containers away from the area around the fire. Dike runoff from fire control for later disposal.

FIRE INVOLVING TANKS, RAIL TANK CARS OR HIGHWAY TANKS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Do not get water inside containers. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks in direct contact with flames. (ERG, 2024)

Use foam, dry powder, carbon dioxide.

If material on fire or involved in fire: Use foam, dry chemical, or carbon dioxide. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Keep run-off water out of sewers and water sources.

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

Flash point: 215 °F (NTP, 1992)

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 Methods and materials for containment and cleaning up

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.

SPILL: Increase the immediate precautionary measure distance, in the downwind direction, as necessary.

FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

Remove all ignition sources. Personal protection: chemical protection suit and filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Collect leaking liquid in covered containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Environmental considerations- land spill: Dig a pit, pond, lagoon, holding area to contain liquid or solid material. /SRP: If time permits, pits, ponds, lagoons, soak holes, or holding areas should be sealed with an impermeable flexible membrane liner./ Cover solids with a plastic sheet to prevent dissolving in rain or fire fighting water. Dike surface flow using soil, sand bags, foamed polyurethane, or foamed concrete.

Environmental considerations- water spill: Use natural barriers or oil spill control booms to Use natural deep water pockets, excavated lagoons, barriers to trap material at bottom. Remove trapped material with suction hoses.

Environmental considerations- air spill: Apply water spray or mist to knock down vapors.

SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.

If material not on fire and not involved in fire: Keep material out of water sources and sewers. Use water spray to knock-down vapors.

Personnel protection: Avoid breathing vapors. Keep upwind. Do not handle broken packages unless wearing appropriate personal protective equipment.

SRP: The scientific literature for the use of contact lenses in industry is conflicting. The benefit or detrimental effects of wearing contact lenses depend not only upon the substance, but also on factors including the form of the substance, characteristics and duration of the exposure, the uses of other eye protection equipment, and the hygiene of the lenses. However, there may be individual substances whose irritating or corrosive properties are such that the wearing of contact lenses would be harmful to the eye. In those specific cases, contact lenses should not be worn. In any event, the usual eye protection equipment should be worn even when contact lenses are in place.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]:

ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Stop leak if you can do it without risk. Prevent entry into waterways, sewers, basements or confined areas. Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers. DO NOT GET WATER INSIDE CONTAINERS. (ERG, 2024)

Cool. Ventilation along the floor. Provision to contain effluent from fire extinguishing. Store in an area without drain or sewer access.

7.2 Conditions for safe storage, including any incompatibilities

Cool. Ventilation along the floor. Provision to contain effluent from fire extinguishing. Store in an area without drain or sewer access.

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

Store in original container. Keep upright to prevent leakage.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

8.1.2 Appropriate engineering controls

Use in a well-ventilated area. Chemical fume hood recommended for powder handling.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear chemical safety goggles.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Respiratory protection usually not required under normal use with adequate ventilation.

Use N95 respirator for large-scale powder handling.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance: Citral appears as a clear yellow colored liquid with a lemon-like odor. Less dense than water and insoluble in water. Toxic by ingestion. Used to make other chemicals.

b) Odor: Strong lemon odor

c) Odor threshold: No data available

d) pH: ACID VALUE: 5.0 MAX

e) Melting point/freezing point: Melting point <-10 °C.

f) Initial boiling point and boiling range: 444 °F at 760 mmHg (Decomposes) (NTP, 1992)

g) Flash point: 215 °F (NTP, 1992)

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: 5 mmHg at 194 °F ; 1 mmHg at 143.1 °F; 760 mmHg at 442 °F (NTP, 1992)

l) Vapor density: No data available

m) Relative density: 0.891 to 0.897 at 59 °F (NTP, 1992)
n) Water solubility: 0.1 to 1 mg/mL at 64 °F (NTP, 1992)
o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 3
p) Auto-ignition temperature: 225 °C
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 information

Topological Polar Surface Area (TPSA): 17.1 Å²
Complexity: 171

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

10.5 Incompatible materials

Strong oxidizing agents, strong acids, strong bases.

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO□).
See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:
No acute toxicity data available.
Skin corrosion/irritation:
Causes skin irritation (H315).
Serious eye damage/eye irritation:
Causes serious eye irritation (H319).
Respiratory or skin sensitization:
May cause an allergic skin reaction (H317).
Germ cell mutagenicity:

No data available.

Carcinogenicity:

No data available.

Reproductive toxicity:

Suspected of damaging fertility or the unborn child (H361).

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

Carcinogen classification:

Citral

TR-505: Toxicology and Carcinogenesis Studies of Citral (Microencapsulated) (CASRN 5392-40-5) in F344/N Rats and B6C3F1 Mice (Feed Studies) (2003)

05/03/01

No Evidence

No Evidence

No Evidence

Equivocal Evidence

Under the conditions of these 2-year feed studies, there was no evidence of carcinogenic activity of citral in male or female F344/N rats exposed to 1,000, 2,000, or 4,000 ppm. There was no evidence of carcinogenic activity of citral in male B6C3F1 mice exposed to 500, 1,000, or

Signs and symptoms of exposure:

Cough.

Redness.

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

LC50 Oryzias latipes (Medaka) 6.1 mg/L/24 hr; semi-static, 21-23 °C, pH 6.9-7.3, dissolved oxygen 4.9-9.1 mg/L /98.9% pure/

LC50 Oryzias latipes (Medaka) 5.8 mg/L/48 hr; semi-static, 21-23 °C, pH 6.9-7.3, dissolved oxygen 4.9-9.1 mg/L /98.9% pure/

LC50 Oryzia latipes (Medaka) 4.1 mg/L 96 hr; semistatic bioassay

LC50 Leuciscus idus 4.6-10 mg/L 96 hr; static bioassay

For more Ecotoxicity Values (Complete) data for CITRAL (8 total), please visit the HSDB record page.

The substance is toxic to aquatic organisms. It is strongly advised not to let the chemical enter into the environment.

Citral's production and use in perfumery, as a flavor, and in chemical synthesis may result in its release to the environment through various waste streams. It is a constituent of many commercial oils such as lemon grass, verbena, lemon, and orange. If released to air, an estimated vapor pressure of 9.13X10-2 mm Hg at 25 °C indicates citral will exist solely as a vapor in the atmosphere. Vapor-phase citral will be degraded in the atmosphere by

reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 3 hrs. Citral does contain chromophores that absorb at wavelengths >290 nm and therefore may be susceptible to direct photolysis by sunlight. If released to soil, citral is expected to have high mobility based upon an estimated Koc of 83. Volatilization from moist soil surfaces is expected to be an important fate process based upon an estimated

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 3

Low potential for bioaccumulation (Log P < 3).

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available.

12.6 Other adverse effects

No other adverse ecological effects identified.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION

14.1 UN number

Not regulated as dangerous goods (research quantities typically exempt).

14.2 UN proper shipping name

Not subject to transport regulations (small quantities for research use).

14.3 Transport hazard class(es)

Not classified as dangerous goods for transport (research quantities).

DOT label: Poison

14.4 Packing group

Not applicable (not regulated as dangerous goods in typical research quantities).

14.5 Environmental hazards

Marine pollutant: No (not classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable.

15. REGULATORY INFORMATION

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

US EPA / TSCA: Subject to EPA TSCA regulations

EU ECHA / REACH: Registered (REACH Active)

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:

Acute (short-term) health hazard

Chronic (long-term) health hazard

Fire hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

California Prop. 65 Components:

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

Other regulatory listings:

- The Australian Inventory of Industrial Chemicals: Chemical: 2,6-Octadienal, 3,7-dimethyl-, (2E)-

- The Australian Inventory of Industrial Chemicals: Chemical: 2,6-Octadienal, 3,7-dimethyl-

- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Fragrance Allergen Authoritative List - Annex III of the EU Cosmetics Regulation No. 1223/2009 - Fragrance Allergens Report - if present in a rinse-off cosmetic product at a concentrat

- EFSA Legal Basis: Regulation (EC) No 1831/2003 (amended)

- Status Regulation (EC): 2004/129/EC

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/09

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product. Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.