ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

trans-Citral = trans-3,7-Dimethyl-octa-2,6-dien-1-al

Revision Date:2023-05-27 Revision Number:1

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

Product identifier

Product name	: trans-Citral = trans-3,7-Dimethyl-octa-2,6-dien-1-al
CBnumber	: CB1875005
CAS	: 141-27-5
EINECS Number	: 205-476-5
Synonyms	: 2,6-Octadienal, 3,7-dimethyl-, (E)-,α-Citral

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

Relevant identified uses	: For R&D use only. Not for medicinal, household or other use.
Uses advised against	: none

Company Identification

Company	: Chemicalbook
Address	: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone	: 400-158-6606

SECTION 2: Hazards identification

Classification of the substance or mixture

Skin irritation, Category 2

Skin sensitization, Sub-category 1B

Eye irritation, Category 2

Label elements

Pictogram(s)

Signal word	Warning

Hazard statement(s)

H315 Causes skin irritation

H317 May cause an allergic skin reaction

H319 Causes serious eye irritation

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P272 Contaminated work clothing should not be allowed out of the workplace.

Response

P302+P352 IF ON SKIN: Wash with plenty of water/...

P321 Specific treatment (see ... on this label).

P332+P317 If skin irritation occurs: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

P333+P317 If skin irritation or rash occurs: Get medical help.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Storage

none

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: trans-Citral = trans-3,7-Dimethyl-octa-2,6-dien-1-al
Synonyms	: 2,6-Octadienal, 3,7-dimethyl-, (E)-,α-Citral
CAS	: 141-27-5
EC number	: 205-476-5
MF	: C10H16O
MW	: 152.23

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest.

Following skin contact

Rinse and then wash skin with water and soap.

Following eye contact

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

Following ingestion

Rinse mouth.

Most important symptoms and effects, both acute and delayed

SYMPTOMS: Symptoms of exposure to this compound may include contact dermatitis. ACUTE/CHRONIC HAZARDS: This compound is a local irritant. When heated to decomposition it emits acrid smoke and fumes. (NTP, 1992)

Indication of any immediate medical attention and special treatment needed

Absorption, Distribution and Excretion

Male Fischer F344 rats were given citral labelled with 14C at the C1 and C2 positions in a single oral dose of 5, 50, or 500 mg/kg bw or an intravenous dose of 5 mg/kg bw. After 72 h, the animals were sacrificed and tissues and excreta analyzed for radioactivity. Most radiolabel was excreted in the urine, feces, and expired air as 14CO2 or [14C]citral within 24 hr, regardless of the dose or route of administration. At the lowest oral dose, 83% of the radiolabel was recovered within 72 hr (51% in urine, 12% in feces, 17% as expired 14CO2, <1% as expired [14C]citral, and 3% in total tissues). Production of 14CO2 essentially ceased 12 hr after treatment, and the amount of 14C found in any tissue was very small (<2%). This excretion profile did not change much with increasing oral dose, although ... oxidation to CO2 was somewhat greater at the lowest dose.

SECTION 5: Firefighting measures

Extinguishing media

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.

Specific Hazards Arising from the Chemical

This chemical is combustible. (NTP, 1992)

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours.Avoid contacting with skin and eye. Use personal protective equipment.Wear chemical impermeable gloves. Ensure adequate ventilation.Remove all sources of ignition. Evacuate personnel to safe areas.Keep people away from and upwind of spill/leak.

Environmental precautions

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.

Methods and materials for containment and cleaning up

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.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

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.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	Oil
Colour	Colourless to Light Yellow
Odour	Strong lemon odor
Melting point/freezing point	< -20 °C. Atm. press.:1 013 hPa.
Boiling point or initial boiling point and	228.77 °C. Atm. press.:1 013.25 hPa. Remarks:Extrapolated value.

boiling range	
Flammability	Combustible.
Lower and upper explosion limit/flammability limit	no data available
Flash point	98 °C. Atm. press.:1 013 hPa.
Auto-ignition temperature	225 °C. Atm. press.:1 013 hPa.
Decomposition temperature	no data available
pH	ACID VALUE: 5.0 MAX
Kinematic viscosity	kinematic viscosity (in mm2/s) = 2.42. Temperature:20°C.;kinematic viscosity (in mm2/s) = 1.67. Temperature:40°C.
Solubility	Chloroform (Slightly), Ethanol (Slightly)
Partition coefficient n-octanol/water	log Pow = 2.76. Temperature:25 °C.
Vapour pressure	0.071 hPa. Temperature:25 °C. Remarks:Extrapolated value.;0.045 hPa. Temperature:20 °C. Remarks:Extrapolated value.
Density and/or relative density	0.887 g/cm3. Temperature:20 °C.;0.871 g/cm3. Temperature:40 °C.
Relative vapour density	(air = 1): 5.3
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on burning. This produces irritating fumes. The substance may polymerize due to heating.

Chemical stability

Not stable to alkalies and strong acids

Possibility of hazardous reactions

CombustibleCITRAL is an aldehyde. Aldehydes are frequently involved in self-condensation or polymerization reactions. These reactions are exothermic; they are often catalyzed by acid. Aldehydes are readily oxidized to give carboxylic acids. Flammable and/or toxic gases are generated by the combination of aldehydes with azo, diazo compounds, dithiocarbamates, nitrides, and strong reducing agents. Aldehydes can react with air to give first peroxo acids, and ultimately carboxylic acids. These autoxidation reactions are activated by light, catalyzed by salts of transition metals, and are autocatalytic (catalyzed by the products of the reaction). The addition of stabilizers (antioxidants) to shipments of aldehydes retards autoxidation. This compound can react with alkalis and strong acids. It can readily isomerize. (NTP, 1992)

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and irritating fumes.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 - rat (male/female) - ca. 6 800 mg/kg bw.
- Inhalation: no data available
- Dermal: LD50 - rat (male/female) - > 2 000 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Leuciscus idus - 6.78 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 6.8 mg/L - 48 h.

Toxicity to algae: EC50 - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - 103.8 mg/L - 72 h.

Toxicity to microorganisms: EC20 - activated sludge, domestic - ca. 68 mg/L - 30 min. Remarks:Respiration rate.

Persistence and degradability

AEROBIC: Citral, present at 100 mg/L, reached 92% of its theoretical BOD in four weeks using an activated sludge inoculum at 30 mg/L and

the Japanese MITI test(1); therefore, this compound is expected to biodegrade rapidly.

Bioaccumulative potential

An estimated BCF of 10 was calculated in fish for citral(SRC), using a water solubility of 1,340 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of citral is estimated as 83(SRC), using a water solubility of 1,340 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that citral is expected to have high mobility in soil.

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

PICCS

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Listed.

Korea Existing Chemicals List (KECL)

Not Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

ECHA - European Chemicals Agency, website: https://echa.europa.eu/

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