MATERIAL SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Date of issue: 02/05/2013 Version 1.0

SECTION 1. Identification

Product identifier

Product number 802489

Product name Citral (mixture of cis- and trans-isomers) for synthesis

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

Identified uses Chemical for synthesis

Details of the supplier of the safety data sheet

Company EMD Millipore Corporation | 290 Concord Road, Billerica, MA 01821, United States of America | SDS Phone Support: +1-978-715-1335 | General Inquiries: +1-978-715-4321 | Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)

e-mail: mm_sds@merckgroup.com

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

SECTION 2. Hazards identification

GHS Classification

Skin irritation, Category 2, H315
Skin sensitization, Category 1, H317

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

GHS-Labeling

Hazard pictograms

Signal Word
Warning

Hazard Statements
H315 Causes skin irritation.
H317 May cause an allergic skin reaction.

Precautionary Statements
P280 Wear protective gloves.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

OSHA Hazards
This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Other hazards
None known.

SECTION 3. Composition/information on ingredients

Formula	$(CH_3)_2C=CHCH_2CH_2C(CH_3)=CHCHO$	$C_{10}H_{16}O$ (Hill)
CAS-No.	5392-40-5	
Molar mass	152.23 g/mol	

Hazardous ingredients
Chemical Name (Concentration)
CAS-No.
citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers) (>= 90 % - <= 100 %)
5392-40-5

SECTION 4. First aid measures

Description of first-aid measures
Inhalation
After inhalation: fresh air.

Skin contact
After skin contact: wash off with plenty of water. Remove contaminated clothing. Consult a physician.

Eye contact
After eye contact: rinse out with plenty of water.

Ingestion
After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed
irritant effects, Allergic reactions, Cough, Shortness of breath, Drowsiness

Indication of any immediate medical attention and special treatment needed
No information available.

SECTION 5. Fire-fighting measures

Extinguishing media
Suitable extinguishing media
Carbon dioxide (CO2), Foam, Dry powder

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.

Special hazards arising from the substance or mixture
Combustible material
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air on intense heating.
Development of hazardous combustion gases or vapors possible in the event of fire.

Advice for firefighters
Special protective equipment for fire-fighters
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information
Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Avoid substance contact. Do not breathe vapors, aerosols. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

Environmental precautions
Do not empty into drains.

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.

SECTION 7. Handling and storage

Precautions for safe handling
Observe label precautions.

Conditions for safe storage, including any incompatibilities
Tightly closed.

Store at +15°C to +25°C (+59°F to +77°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Ingredients

Basis	Value	Threshold limits	Remarks
citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers) 5392-40-5			
ACGIH	Time Weighted Average (TWA):	5 ppm	Form of exposure: Inhalable fraction and vapor.
	Skin designation:		Can be absorbed through the skin. Form of exposure: Inhalable fraction and vapor.

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

Eye/face protection

Safety glasses

Hand protection

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Other protective equipment:

protective clothing

Respiratory protection

required when vapors/aerosols are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

SECTION 9. Physical and chemical properties

Physical state	liquid
Color	light yellow
Odor	of lemons
Odor Threshold	No information available.
pH	No information available.

Melting point	< -20 °C
Boiling point/boiling range	441 - 444 °F (227 - 229 °C) at 1,013 hPa
Flash point	208 °F (98 °C) Method: DIN 51758
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	4.3 %(V)
Upper explosion limit	9.9 %(V)
Vapor pressure	< 1 hPa at 122 °F (50 °C)
Relative vapor density	5.26 (Lit.)
Relative density	0.89 g/cm³ at 68 °F (20 °C)
Water solubility	0.42 g/l at 77 °F (25 °C)
Partition coefficient: n-octanol/water	log Pow: 2.76 (25 °C) OECD Test Guideline 107 Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	> 374 °F (> 190 °C)
Viscosity, dynamic	No information available.
Explosive properties	No information available.
Ignition temperature	437 °F (225 °C) Method: DIN 51794

SECTION 10. Stability and reactivity

Reactivity

Forms explosive mixtures with air on intense heating.

Chemical stability

Sensitivity to light
Sensitive to air.

Possibility of hazardous reactions

Violent reactions possible with:

Aluminum, alkalines, Strong oxidizing agents, acids

Conditions to avoid

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

Incompatible materials

Aluminum, Mild steel

Hazardous decomposition products

no information available

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure
Eye contact, Skin contact

Acute oral toxicity
LD50 rat: 4,950 mg/kg (IUCLID)

absorption

Acute inhalation toxicity

Symptoms: Possible damages:, mucosal irritations

Acute dermal toxicity
LD50 rabbit: 2,250 mg/kg
(IUCLID)

Skin irritation
rabbit
Result: Irritations
(IUCLID)

Causes skin irritation.

Eye irritation
rabbit
Result: No eye irritation
(IUCLID)

Sensitization
Sensitization test (Magnusson and Kligman):
Result: positive
(IUCLID)

May cause an allergic skin reaction.

Genotoxicity in vitro
Mutagenicity (mammal cell test): chromosome aberration.
Result: negative
(National Toxicology Program)

Ames test
Result: negative
(National Toxicology Program)

Specific target organ systemic toxicity - single exposure
The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ systemic toxicity - repeated exposure
The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard
Regarding the available data the classification criteria are not fulfilled.

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.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
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.
ACGIH	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information
Systemic effects:
After absorption:
Drowsiness
Further data:
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish
LC50 Leuciscus idus (Golden orfe): > 4.6 - 10 mg/l; 96 h
DIN 38412 part 15 (External MSDS)

Toxicity to daphnia and other aquatic invertebrates
EC50 Daphnia magna (Water flea): 7 mg/l; 48 h (External MSDS)

Toxicity to algae
IC50 Desmodesmus subspicatus (green algae): 16 mg/l; 72 h (IUCLID)

Toxicity to bacteria
EC50 Pseudomonas putida: 2,100 mg/l; 30 min (External MSDS)

Persistence and degradability
Biodegradability
> 90 %; 28 d
OECD Test Guideline 301C
Readily biodegradable.

Bioaccumulative potential
Partition coefficient: n-octanol/water
log Pow: 2.76 (25 °C)
OECD Test Guideline 107
Bioaccumulation is not expected (log Pow <1).

Mobility in soil
No information available.

Other adverse effects
Additional ecological information
Biological effects:
When discharged properly, no impairments in the function of adapted biological wastewater treatment plants are to be expected.
Further information on ecology
Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)
Not classified as dangerous in the meaning of transport regulations.

Air transport (IATA)
Not classified as dangerous in the meaning of transport regulations.

Sea transport (IMDG)
Not classified as dangerous in the meaning of transport regulations.

SECTION 15. Regulatory information

United States of America

OSHA Hazards
Skin irritant
Skin sensitizer

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

SARA 311/312 Hazards
Acute Health Hazard

SARA 313
SARA 313: 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 302
SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

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

Pennsylvania Right To Know
Ingredients
citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers)

New Jersey Right To Know
Ingredients
citral; 3,7-dimethyl-2,6-octadienal (cis-/trans-mixture of isomers)

Notification status

TSCA:	On TSCA Inventory
DSL:	All components of this product are on the Canadian DSL.

SECTION 16. Other information

Training advice
Provide adequate information, instruction and training for operators.

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

H315	Causes skin irritation.
H317	May cause an allergic skin reaction.

Key or legend to abbreviations and acronyms used in the safety data sheet
Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Date of issue:02/05/2013