

SAFETY DATA SHEET

Version 6.8
Revision Date 08/05/2024
Print Date 08/06/2024

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

1.1 Product identifiers

Product name : Safranal

Product Number : W338907

Brand : Aldrich

CAS-No. : 116-26-7

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 sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +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
Acute toxicity, Oral (Category 4), H302
Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319

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Skin sensitization (Sub-category 1A), H317
Short-term (acute) aquatic hazard (Category 2), H401
Long-term (chronic) aquatic hazard (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 Statements

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

Precautionary Statements

P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P261	Avoid breathing mist or vapors.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
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.
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.
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 + 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

Synonyms : 2,3-Dihydro-2,2,6-trimethylbenzaldehyde

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Formula : C₁₀H₁₄O
Molecular weight : 150.22 g/mol
CAS-No. : 116-26-7
EC-No. : 204-133-7

Component	Classification	Concentration
2,3-Dihydro-2,2,6-trimethylbenzaldehyde		
	Flam. Liq. 4; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; Skin Sens. 1A; Aquatic Acute 2; Aquatic Chronic 2; H227, H302, H315, H319, H317, H401, H411	<= 100 %

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

No data available

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

No data available

5.2 Special hazards arising from the substance or mixture

Carbon oxides
Combustible.

5.3 Advice for firefighters

No data available

5.4 Further information

No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For personal protection see section 8.

6.2 Environmental precautions

No data available

6.3 Methods and materials for containment and cleaning up

No data available

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

No data available

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

No data available

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|--|--|
| a) Appearance | Form: clear, liquid
Color: yellow |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/freezing point: < -20 °C (< -4 °F) at ca.1,013 hPa
- Regulation (EC) No. 440/2008, Annex, A.1 |
| f) Initial boiling point and boiling range | 70 °C 158 °F at 1 hPa - lit. |
| g) Flash point | 86 °C (187 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, | No data available |

gas)	
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	0.103 hPa at 20 °C (68 °F) - OECD Test Guideline 104
l) Vapor density	No data available
m) Density	0.966 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	514.9 g/l at 20 °C (68 °F) - OECD Test Guideline 105
o) Partition coefficient: n-octanol/water	log Pow: 2.7 at 35 °C (95 °F) - OECD Test Guideline 117 - Bioaccumulation is not expected.
p) Autoignition temperature	282 °C (540 °F) at 962 hPa
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

Surface tension	59.4 mN/m at 20 °C (68 °F) - OECD Test Guideline 115
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SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

No data available

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong acids

Strong bases

Strong oxidizing agents

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

No data available

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 - female - > 300 - < 2,000 mg/kg

(OECD Test Guideline 423)

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Skin - EPISKIN Human Skin Model Test

Result: irritating - 42 h

(OECD Test Guideline 439)

Serious eye damage/eye irritation

Eyes - chicken

Result: Irritating to eyes.

(OECD Test Guideline 438)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: positive

Remarks: (ECHA)

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

Test Type: in vitro test

Test system: human lymphoblastoid cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 487

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 490

Result: negative

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 - Gavage - NOAEL (No observed adverse effect level) - 125 mg/kg

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	semi-static test LC50 - Danio rerio (zebra fish) - 4.3 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia - 22.73 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata - 15.5 mg/l - 72 h (OECD Test Guideline 201) static test NOEC - Pseudokirchneriella subcapitata - < 1 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - Sewage sludge - > 100 mg/l - 3 h (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 0 % - Not readily biodegradable.
(OECD Test Guideline 301F)

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

No data available

SECTION 14: Transport information

DOT (US)

NA-Number: 1993 Class: NONE Packing group: III
Proper shipping name: Combustible liquid, n.o.s. (2,3-Dihydro-2,2,6-trimethylbenzaldehyde)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

Not dangerous goods

IATA

Not dangerous goods

SECTION 15: Regulatory information

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

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

SARA 311/312 Hazards : Fire Hazard
Acute Health Hazard

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.

US State Regulations

Massachusetts Right To Know

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

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Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

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