
1. PRODUCT AND COMPANY IDENTIFICATION**1.1 Product identifiers**

Product name : 3,5,5-Trimethyl-1-hexanol

Product Number : W332402

Brand : Aldrich

CAS-No. : 3452-97-9

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 sheetCompany : Sigma-Aldrich Inc.
3050 Spruce Street
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

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

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

Specific target organ toxicity - repeated exposure, Oral (Category 2), H373

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.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H373	May cause damage to organs through prolonged or repeated exposure if swallowed.
H411	Toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P260	Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
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.
P314	Get medical advice/ attention if you feel unwell.
P321	Specific treatment (see supplemental first aid instructions on this label).
P332 + P313	If skin irritation 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 for extinction.
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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Molecular weight	:	144.25 g/mol
CAS-No.	:	3452-97-9
EC-No.	:	222-376-7

Hazardous components

Component	Classification	Concentration
3,5,5-Trimethyl-1-hexanol		
	Flam. Liq. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT RE 2; Aquatic Acute 2; Aquatic Chronic 2; H227, H315, H319, H373, H411	<= 100 %

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**

For small (incipient) fires, use media such as "alcohol" foam, dry chemica as far as possible. Use very large quantities (flooding) of water applied ineffective. Cool all affected containers with flooding quantities of wat

5.2 Special hazards arising from the substance or mixture

Carbon oxides

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 an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local 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.

Storage class (TRGS 510): 10: Combustible liquids

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

Contains no substances with occupational exposure limit values.

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
Colour: colourless |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | 5.9 - 6.1 at 25 °C (77 °F) |
| e) Melting point/freezing point | Melting point/range: < -60 °C (< -76 °F)
Melting point/range: -30 °C (-22 °F) |

- | | |
|---|--|
| f) Initial boiling point and boiling range | 193 - 194 °C (379 - 381 °F) - lit. |
| g) Flash point | 80 °C (176 °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 | 24 hPa at 100 °C (212 °F)
0.0901 hPa at 25 °C (77 °F) |
| l) Vapour density | No data available |
| m) Relative density | 0.824 g/mL at 25 °C (77 °F) |
| n) Water solubility | 0.45 g/l at 25 °C (77 °F) |
| o) Partition coefficient: n-octanol/water | log Pow: 3.026 |
| p) Auto-ignition temperature | No data available |
| 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 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

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 - 2,980 - 6,400 mg/kg

LD50 Oral - Rat - 3,160 mg/kg

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Moderate skin irritation
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Moderate eye irritation
(OECD Test Guideline 405)

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

Ames test

S. typhimurium
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.

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

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 on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Ingestion - May cause damage to organs through prolonged or repeated exposure.

Gavage - Kidney

Aspiration hazard

No data available

Additional Information

Repeated dose toxicity - Rat - female - Gavage

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 fish

LC50 - Pimephales promelas (fathead minnow) - 5.7 mg/l - 96 h(3,5,5-Trimethyl-1-hexanol)

LC50 - Pimephales promelas (fathead minnow) - 28.2 mg/l - 96 h(3,5,5-Trimethyl-1-hexanol)

LC50 - Carassius auratus (goldfish) - 16 mg/l - 24 h(3,5,5-Trimethyl-1-hexanol)
(OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates Immobilization EC50 - Daphnia (water flea) - 6.77 mg/l - 48 h(3,5,5-Trimethyl-1-hexanol)

Toxicity to algae Growth inhibition EC50 - Algae - 33.3 mg/l - 72 h(3,5,5-Trimethyl-1-hexanol) (OECD Test Guideline 201)

12.2 Persistence and degradability

Biodegradability Result: - According to the results of tests of biodegradability this product is not readily biodegradable.

12.3 Bioaccumulative potential

Bioaccumulation Cyprinus carpio (Carp) - 42 d (3,5,5-Trimethyl-1-hexanol)

Bioconcentration factor (BCF): 3.9 - 8.1

12.4 Mobility in soil

Adsorbs on soil.(3,5,5-Trimethyl-1-hexanol)

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.

Avoid release to the environment.

Stability in water pH 4.7 - 9 at 50 °C(3,5,5-Trimethyl-1-hexanol)
Remarks: Hydrolyses slowly.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company. 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. (3,5,5-Trimethyl-1-hexanol)
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. (3,5,5-Trimethyl-1-hexanol)
Marine pollutant : yes

IATA

UN number: 3082 Class: 9 Packing group: III
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (3,5,5-Trimethyl-1-hexanol)

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

	CAS-No.	Revision Date
3,5,5-Trimethyl-1-hexanol	3452-97-9	1993-04-24

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
3,5,5-Trimethyl-1-hexanol	3452-97-9	1993-04-24

New Jersey Right To Know Components

	CAS-No.	Revision Date
3,5,5-Trimethyl-1-hexanol	3452-97-9	1993-04-24

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.

H227	Combustible liquid.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H373	May cause damage to organs through prolonged or repeated exposure if swallowed.
H401	Toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.

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

Copyright 2016 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only. The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956
Version: 6.0

Revision Date: 05/26/2018

Print Date: 11/16/2018