



3,5,5-Trimethyl hexanol

synerzine™

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 06/05/2015

Version: 1.0

SECTION 1: Identification

1.1. Identification

Product form	: Substance
Substance name	: 3,5,5-Trimethyl hexanol
Chemical name	: 3,5,5-Trimethylhexan-1-ol
CAS-No.	: 3452-97-9
Product code	: (US) W0240
Formula	: C9H20O
Synonyms	: 3,5,5-Trimethylhexanol / TRIMETHYLHEXANOL / Trimethylhexanol, 3,5,5- / 3,5,5-Trimethylhexan-1-ol / 3,5,5-Trimethyl-1-hexanol / Hexanol, 3,5,5-trimethyl-

1.2. Recommended use and restrictions on use

Use of the substance/mixture : Flavor and/or Fragrance

1.3. Supplier

Synerzine
5340 Hwy 42 S
Ellenwood, Georgia 30294 - USA
T 404-524-6744 - F 404-577-1651
info@synerzine.com - www.synerzine.com

1.4. Emergency telephone number

Emergency number : Infotrac 1-800-535-5053 (Contract# 102471) Dial +1-352-323-3500 when outside the US

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS-US classification

Flammable liquids Category 4	H227	Combustible liquid
Skin corrosion/irritation Category 2	H315	Causes skin irritation
Serious eye damage/eye irritation Category 2A	H319	Causes serious eye irritation
Specific target organ toxicity (repeated exposure) Category 2	H373	May cause damage to organs (Not classified) through prolonged or repeated exposure (Not classified)
Hazardous to the aquatic environment - Acute Hazard Category 2	H401	Toxic to aquatic life
Hazardous to the aquatic environment - Chronic Hazard Category 2	H411	Toxic to aquatic life with long lasting effects

Full text of H statements : see section 16

2.2. GHS Label elements, including precautionary statements

GHS-US labeling

Hazard pictograms (GHS-US) :



Signal word (GHS-US) :

Warning

Hazard statements (GHS-US) :

H227 - Combustible liquid
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H373 - May cause damage to organs (Not classified) through prolonged or repeated exposure (Not classified)
H401 - Toxic to aquatic life
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Precautionary statements (GHS-US) : P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. heat, hot surfaces, open flames, sparks
P260 - Do not breathe fume, gas, spray, vapors.
P264 - Wash hands, forearms and face thoroughly after handling.
P273 - Avoid release to the environment.
P280 - Wear eye protection, face protection, protective clothing, protective gloves.
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 alcohol resistant foam, dry sand 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. Other hazards which do not result in classification

No additional information available

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/Information on ingredients

3.1. Substances

Name	Product identifier	%	GHS-US classification
3,5,5-Trimethyl hexanol (Main constituent)	(CAS-No.) 3452-97-9	85 - 100	Flam. Liq. 4, H227 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT RE 2, H373 Aquatic Acute 2, H401 Aquatic Chronic 2, H411

Full text of hazard classes and H-statements : see section 16

3.2. Mixtures

Not applicable

SECTION 4: First-aid measures

4.1. Description of first aid measures

First-aid measures general : Get medical advice/attention if you feel unwell.
First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing.
First-aid measures after skin contact : Wash skin with plenty of water. Take off contaminated clothing. If skin irritation occurs: Get medical advice/attention.
First-aid measures after eye contact : Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.
First-aid measures after ingestion : Call a poison center/doctor/physician if you feel unwell.

4.2. Most important symptoms and effects (acute and delayed)

Symptoms/effects after skin contact : Irritation.
Symptoms/effects after eye contact : Eye irritation.

4.3. Immediate medical attention and special treatment, if necessary

Treat symptomatically.

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media : Water spray. Dry powder. Foam. Carbon dioxide.

5.2. Specific hazards arising from the chemical

Fire hazard : Combustible liquid.
Reactivity : The product is non-reactive under normal conditions of use, storage and transport.

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5.3. Special protective equipment and precautions for fire-fighters

Protection during firefighting : Do not attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Ventilate spillage area. No open flames, no sparks, and no smoking. Do not breathe fume, gas, mist, spray, vapors. Avoid contact with skin and eyes.

6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".

6.2. Environmental precautions

Avoid release to the environment.

6.3. Methods and material for containment and cleaning up

For containment : Collect spillage.

Methods for cleaning up : Take up liquid spill into absorbent material. Notify authorities if product enters sewers or public waters.

Other information : Dispose of materials or solid residues at an authorized site.

6.4. Reference to other sections

For further information refer to section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Ensure good ventilation of the work station. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Wear personal protective equipment. Do not breathe fume, gas, mist, spray, vapors. Avoid contact with skin and eyes.

Hygiene measures : Wash contaminated clothing before reuse. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store in a well-ventilated place. Keep cool.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Appropriate engineering controls

Appropriate engineering controls : Ensure good ventilation of the work station.

Environmental exposure controls : Avoid release to the environment.

8.3. Individual protection measures/Personal protective equipment

Hand protection:

Protective gloves

Eye protection:

Safety glasses

Skin and body protection:

Wear suitable protective clothing

Respiratory protection:

In case of insufficient ventilation, wear suitable respiratory equipment

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SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Appearance	: Colorless oily liquid.
Color	: colorless
Odor	: strong oily-herbaceous odor
Odor threshold	: No data available
pH	: No data available
Melting point	: Not applicable
Freezing point	: No data available
Boiling point	: 193 °C
Flash point	: 176 °F (open cup)
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: Not applicable.
Vapor pressure	: 24 hPa (at 100 °C)
Relative vapor density at 20 °C	: No data available
Relative density	: No data available
Specific gravity / density	: 0.829 g/cm ³ (at 20 °C)
Solubility	: acetone. Ether. Slightly soluble in water. soluble in alcohols.
Log Pow	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosion limits	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

Avoid contact with hot surfaces. Heat. No flames, no sparks. Eliminate all sources of ignition.

10.5. Incompatible materials

No additional information available

10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

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LD50 oral rat	1160 mg/kg
LD50 dermal rabbit	2990 mg/kg

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3,5,5-Trimethyl hexanol (3452-97-9)	
ATE US (oral)	1160 mg/kg body weight
ATE US (dermal)	2990 mg/kg body weight

Skin corrosion/irritation	: Causes skin irritation.
Serious eye damage/irritation	: Causes serious eye irritation.
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
Reproductive toxicity	: Not classified
Specific target organ toxicity – single exposure	: Not classified
Specific target organ toxicity – repeated exposure	: May cause damage to organs (Not classified) through prolonged or repeated exposure (Not classified).
Aspiration hazard	: Not classified
Symptoms/effects after skin contact	: Irritation.
Symptoms/effects after eye contact	: Eye irritation.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : Toxic to aquatic life with long lasting effects. Toxic to aquatic life.

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LC50 fish 1	5.7 mg/l (Exposure time: 96 h - Species: Pimephales promelas)
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12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

No additional information available

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Disposal methods

Waste treatment methods : Dispose of contents/container in accordance with licensed collector's sorting instructions.

SECTION 14: Transport information

Department of Transportation (DOT)


In accordance with DOT

Transport document description	: NA1993 Combustible liquid, n.o.s., 3, III
UN-No.(DOT)	: NA1993
Proper Shipping Name (DOT)	: Combustible liquid, n.o.s.
Class (DOT)	: 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120
Packing group (DOT)	: III - Minor Danger
Dangerous for the environment	: Yes

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Marine pollutant	: Yes
	
DOT Packaging Non Bulk (49 CFR 173.xxx)	: 203
DOT Packaging Bulk (49 CFR 173.xxx)	: 241
DOT Symbols	: D - Proper shipping name for domestic use only, or to and from Canada, G - Identifies PSN requiring a technical name
DOT Special Provisions (49 CFR 172.102)	: IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672). T1 - 1.5 178.274(d)(2) Normal..... 178.275(d)(2) T4 - 2.65 178.274(d)(2) Normal..... 178.275(d)(3) TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling = $97 / 1 + a (tr - tf)$ Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling.
DOT Packaging Exceptions (49 CFR 173.xxx)	: 150
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	: 60 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	: 220 L
DOT Vessel Stowage Location	: A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.
Other information	: No supplementary information available.

Transportation of Dangerous Goods

Transport by sea

Transport document description (IMDG)	: UN 3082 ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S., 9, III
UN-No. (IMDG)	: 3082
Proper Shipping Name (IMDG)	: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.
Class (IMDG)	: 9 - Miscellaneous dangerous substances and articles
Packing group (IMDG)	: III - substances presenting low danger
Limited quantities (IMDG)	: 5 L
Marine pollutant	: Yes



Air transport

Transport document description (IATA)	: UN 3082 Environmentally hazardous substance, liquid, n.o.s., 9, III
UN-No. (IATA)	: 3082
Proper Shipping Name (IATA)	: Environmentally hazardous substance, liquid, n.o.s.
Class (IATA)	: 9 - Miscellaneous Dangerous Goods
Packing group (IATA)	: III - Minor Danger

SECTION 15: Regulatory information

15.1. US Federal regulations

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Listed on the United States TSCA (Toxic Substances Control Act) inventory

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15.2. International regulations

CANADA

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Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

3,5,5-Trimethyl hexanol (3452-97-9)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

National regulations

3,5,5-Trimethyl hexanol (3452-97-9)

Listed on the AICS (Australian Inventory of Chemical Substances)
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)
Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory
Listed on the Japanese ISHL (Industrial Safety and Health Law)
Listed on the Korean ECL (Existing Chemicals List)
Listed on NZIoC (New Zealand Inventory of Chemicals)
Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)
Japanese Pollutant Release and Transfer Register Law (PRTR Law)
Listed on the TCSI (Taiwan Chemical Substance Inventory)

15.3. US State regulations

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State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - Pennsylvania - RTK (Right to Know) List
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SECTION 16: Other information

Full text of H-phrases:

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

NFPA health hazard

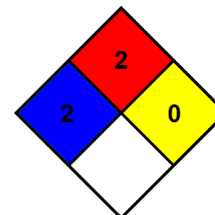
: 2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.

NFPA fire hazard

: 2 - Materials that must be moderately heated or exposed to relatively high ambient temperatures before ignition can occur.

NFPA reactivity

: 0 - Material that in themselves are normally stable, even under fire conditions.



Hazard Rating

Health

: 2 Moderate Hazard - Temporary or minor injury may occur

Flammability

: 2 Moderate Hazard - Materials which must be moderately heated or exposed to high ambient temperatures before ignition will occur. Includes liquids having a flash point at or above 100 F but below 200 F. (Classes II & IIIA)

Physical

: 0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

Personal protection

: C
C - Safety glasses, Gloves, Synthetic apron

Synergism US

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product