

ACR47561

## 3,5,5-Trimethyl-1-hexanol

### SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明: Product Description:	3,5,5-三甲基-1-己醇 3,5,5-Trimethyl-1-hexanol
Cat No. :	475610000; 475610250; 475611000
CAS No	3452-97-9
Molecular Formula	C9 H20 O
Supplier	<b>UK entity/business name</b> Fisher Scientific UK Bishop Meadow Road, Loughborough, Leicestershire LE11 5RG, United Kingdom  <b>EU entity/business name</b> Thermo Fisher Scientific Janssen Pharmaceuticaaan 3a, 2440 Geel, Belgium
Emergency Telephone Number	For information <b>US</b> call: 001-800-227-6701 / <b>Europe</b> call: +32 14 57 52 11 Emergency Number <b>US</b> :001-201-796-7100 / <b>Europe</b> : +32 14 57 52 99 <b>CHEMTREC</b> Tel. No. <b>US</b> :001-800-424-9300 / <b>Europe</b> :001-703-527-3887
E-mail address	begel.sdsdesk@thermofisher.com
Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

### SECTION 2. HAZARD IDENTIFICATION

<b>Physical State</b> Liquid	<b>Appearance</b> No information available	<b>Odor</b> No information available
<b>Emergency Overview</b> Combustible liquid. May be harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. May cause damage to organs through prolonged or repeated exposure.		

#### Classification of the substance or mixture

Flammable liquids.	Category 4
Acute Dermal Toxicity	Category 5
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (repeated exposure)	Category 2

#### Label Elements



**Signal Word****Warning****Hazard Statements**

H227 - Combustible liquid

H313 - May be harmful in contact with skin

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H373 - May cause damage to organs through prolonged or repeated exposure

**Precautionary Statements****Prevention**

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

P264 - Wash face, hands and any exposed skin thoroughly after handling

P280 - Wear protective gloves/protective clothing/eye protection/face protection

**Response**

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

P332 + P313 - If skin irritation occurs: Get medical advice/attention

P337 + P313 - If eye irritation persists: Get medical advice/attention

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

P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish

**Storage**

P403 + P235 - Store in a well-ventilated place. Keep cool

**Disposal**

P501 - Dispose of contents/ container to an approved waste disposal plant

**Physical and Chemical Hazards**

Combustible material.

**Health Hazards**

May be harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. May cause damage to organs through prolonged or repeated exposure.

**Environmental hazards**

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants.

This product does not contain any known or suspected endocrine disruptors. Toxic to terrestrial vertebrates.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Component	CAS No	Weight %
1-Hexanol, 3,5,5-trimethyl-	3452-97-9	<=100

**SECTION 4. FIRST AID MEASURES****General Advice**

If symptoms persist, call a physician.

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

**Inhalation**

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

**Ingestion**

Clean mouth with water and drink afterwards plenty of water.

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**Most important symptoms and effects**

None reasonably foreseeable. . Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

**Self-Protection of the First Aider**

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

**Notes to Physician**

Treat symptomatically.

**SECTION 5. FIRE-FIGHTING MEASURES****Suitable Extinguishing Media**

Water mist may be used to cool closed containers.

**Extinguishing media which must not be used for safety reasons**

No information available.

**Specific Hazards Arising from the Chemical**

Combustible material. Containers may explode when heated.

**Protective Equipment and Precautions for Firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

**SECTION 6. ACCIDENTAL RELEASE MEASURES****Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.

**Environmental Precautions**

Do not flush into surface water or sanitary sewer system.

**Methods for Containment and Clean Up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE****Handling**

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition.

**Storage**

Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters**

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**Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours

**Exposure Controls****Engineering Measures**

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

**Personal protective equipment**

**Eye Protection** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

**Skin and body protection** Long sleeved clothing

**Respiratory Protection** When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.  
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

**Large scale/emergency use** Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced  
**Recommended Filter type:** Organic gases and vapours filter Type A Brown conforming to EN14387

**Small scale/Laboratory use** Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.  
**Recommended half mask:-** Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141  
When RPE is used a face piece Fit Test should be conducted

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice.

**Environmental exposure controls** Prevent product from entering drains. Do not allow material to contaminate ground water system.

**SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

**Appearance**  
**Physical State**

Liquid

**Odor**

No information available

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<b>Odor Threshold</b>	No data available	
<b>pH</b>	Not applicable	
<b>Melting Point/Range</b>	No data available	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	193 °C / 379.4 °F	
<b>Flash Point</b>	79 °C / 174.2 °F	<b>Method -</b> No information available
<b>Evaporation Rate</b>	No data available	
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	
<b>Vapor Pressure</b>	No data available	
<b>Vapor Density</b>	No data available	(Air = 1.0)
<b>Specific Gravity / Density</b>	No data available	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Water Solubility</b>	No information available	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Component</b>	<b>log Pow</b>	
1-Hexanol, 3,5,5-trimethyl-	3.7	
<b>Autoignition Temperature</b>	404 °C / 759.2 °F	
<b>Decomposition Temperature</b>	No data available	
<b>Viscosity</b>	No data available	
<b>Explosive Properties</b>	No information available	explosive air/vapour mixtures possible
<b>Oxidizing Properties</b>	No information available	
<b>Molecular Formula</b>	C9 H20 O	
<b>Molecular Weight</b>	144.26	

## SECTION 10. STABILITY AND REACTIVITY

<b>Stability</b>	Stable under normal conditions.
<b>Hazardous Reactions</b>	None under normal processing.
<b>Hazardous Polymerization</b>	No information available.
<b>Conditions to Avoid</b>	Keep away from open flames, hot surfaces and sources of ignition.
<b>Materials to avoid</b>	No information available.

Hazardous Decomposition Products Carbon oxides.

## SECTION 11. TOXICOLOGICAL INFORMATION

## Product Information

## (a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
1-Hexanol, 3,5,5-trimethyl-	LD50 = 1160 mg/kg ( Rat )	LD50 = 2990 mg/kg ( Rabbit )	

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

## (d) respiratory or skin sensitization;

<b>Respiratory</b>	No data available
<b>Skin</b>	No data available

## 3,5,5-Trimethyl-1-hexanol

(e) germ cell mutagenicity;	No data available
(f) carcinogenicity;	No data available There are no known carcinogenic chemicals in this product
(g) reproductive toxicity;	No data available
(h) STOT-single exposure;	No data available
(i) STOT-repeated exposure;	Category 2
Target Organs	No information available.
(j) aspiration hazard;	No data available

**Symptoms / effects, both acute and delayed** Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

## SECTION 12. ECOLOGICAL INFORMATION

**Ecotoxicity effects** Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
1-Hexanol, 3,5,5-trimethyl-	LC50: = 5.7 mg/L, 96h (Pimephales promelas)			

**Persistence and Degradability**  
**Persistence** No information available  
**Degradation in sewage treatment plant** Persistence is unlikely.  
Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

**Bioaccumulative Potential** Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
1-Hexanol, 3,5,5-trimethyl-	3.7	No data available

**Mobility in soil** No information available

**Endocrine Disruptor Information** This product does not contain any known or suspected endocrine disruptors  
**Persistent Organic Pollutant** This product does not contain any known or suspected substance  
**Ozone Depletion Potential** This product does not contain any known or suspected substance

## SECTION 13. DISPOSAL CONSIDERATIONS

**Waste from Residues/Unused Products** Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

**Contaminated Packaging** Dispose of this container to hazardous or special waste collection point.

## 3,5,5-Trimethyl-1-hexanol

## Other Information

Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

## SECTION 14. TRANSPORT INFORMATION

## Road and Rail Transport

Not Regulated

## IMDG/IMO

Not regulated

## IATA

Not regulated

## Special Precautions for User

No special precautions required

## SECTION 15. REGULATORY INFORMATION

## International Inventories

China, X = listed, Australia, U.S.A. (TSCA), Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Australia (AICS), Korea (KECL), China (IECSC), Japan (ENCS), Philippines (PICCS), Taiwan (TCSI), Japan (ISHL), New Zealand (NZIoC), Japan (ISHL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
1-Hexanol, 3,5,5-trimethyl-	-	-	X	X	222-376-7	X	X	X	X	X	X	KE-34566

## National Regulations

## SECTION 16. OTHER INFORMATION

## Creation Date

27-Jun-2023

## Revision Date

20-Apr-2024

## Revision Summary

SDS sections updated.

## Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

## Legend

**CAS** - Chemical Abstracts Service**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances**PICCS** - Philippines Inventory of Chemicals and Chemical Substances**IECSC** - Chinese Inventory of Existing Chemical Substances**KECL** - Korean Existing and Evaluated Chemical Substances**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List**ENCS** - Japanese Existing and New Chemical Substances**AICS** - Australian Inventory of Chemical Substances**NZIoC** - New Zealand Inventory of Chemicals

## 3,5,5-Trimethyl-1-hexanol

**WEL** - Workplace Exposure Limit  
**ACGIH** - American Conference of Governmental Industrial Hygienists  
**DNEL** - Derived No Effect Level  
**RPE** - Respiratory Protective Equipment  
**LC50** - Lethal Concentration 50%  
**NOEC** - No Observed Effect Concentration  
**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average  
**IARC** - International Agency for Research on Cancer  
**PNEC** - Predicted No Effect Concentration  
**LD50** - Lethal Dose 50%  
**EC50** - Effective Concentration 50%  
**POW** - Partition coefficient Octanol:Water  
**vPvB** - very Persistent, very Bioaccumulative

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association  
**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road  
**OECD** - Organisation for Economic Co-operation and Development  
**BCF** - Bioconcentration factor

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code  
**MARPOL** - International Convention for the Prevention of Pollution from Ships  
**ATE** - Acute Toxicity Estimate  
**VOC** - (Volatile Organic Compound)

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>  
Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**Disclaimer**

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**End of Safety Data Sheet**