

ALFAAL13360

## 3,5,5-Trimethylhexanoic acid

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

产品说明: 3,5,5-三甲基己酸  
Product Description: 3,5,5-Trimethylhexanoic acid

Cat No. : L13360  
CAS No 3302-10-1  
Molecular Formula C9 H18 O2

Supplier Avocado Research Chemicals Ltd.  
(Part of Thermo Fisher Scientific)  
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Recommended Use Laboratory chemicals.  
Uses advised against No Information available

### SECTION 2. HAZARD IDENTIFICATION

**Physical State**  
Liquid

**Appearance**  
Colorless

**Odor**  
Odorless

**Emergency Overview**

Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

#### Classification of the substance or mixture

|                                                    |            |
|----------------------------------------------------|------------|
| Skin Corrosion/Irritation                          | Category 2 |
| Serious Eye Damage/Eye Irritation                  | Category 2 |
| Specific target organ toxicity - (single exposure) | Category 3 |

#### Label Elements



Signal Word

Warning

Hazard Statements

## 3,5,5-Trimethylhexanoic acid

H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation

**Precautionary Statements****Prevention**

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P264 - Wash face, hands and any exposed skin thoroughly after handling  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear protective gloves/protective clothing/eye protection/face protection

**Response**

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P312 - Call a POISON CENTER or doctor if you feel unwell  
P362 + P364 - Take off contaminated clothing and wash it before reuse

**Storage**

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

**Disposal**

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

**Physical and Chemical Hazards**

None identified.

**Health Hazards**

Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

**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.

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

| Component                       | CAS No    | Weight % |
|---------------------------------|-----------|----------|
| Hexanoic acid, 3,5,5-trimethyl- | 3302-10-1 | <=100    |

**SECTION 4. FIRST AID MEASURES****Eye Contact**

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

**Skin Contact**

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.

**Inhalation**

Remove from exposure, lie down. Remove to fresh air.

**Ingestion**

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Drink plenty of water. If possible drink milk afterwards.

**Most important symptoms and effects**

No information available.

**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**

## 3,5,5-Trimethylhexanoic acid

Treat symptomatically.

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

Water spray. Carbon dioxide (CO<sub>2</sub>). Dry chemical. Alcohol resistant foam.

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

No information available.

**Specific Hazards Arising from the Chemical**

Thermal decomposition can lead to release of irritating gases and vapors.

**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. Thermal decomposition can lead to release of irritating gases and vapors.

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

Ensure adequate ventilation.

**Environmental Precautions**

See Section 12 for additional Ecological Information.

**Methods for Containment and Clean Up**

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Sweep up and shovel into suitable containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

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

Avoid contact with skin and eyes. Avoid contact with skin and clothing. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Avoid breathing vapors or mists. Do not ingest. If swallowed then seek immediate medical assistance. Wash thoroughly after handling.

**Storage**

Keep in a dry, cool and well-ventilated place. Keep container tightly closed.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters****Exposure Controls****Engineering Measures**

Ventilation systems. Ensure that eyewash stations and safety showers are close to the workstation location. 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.

## 3,5,5-Trimethylhexanoic acid

## Personal protective equipment

**Eye Protection** Wear safety glasses with side shields (or goggles) Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

| Glove material | Breakthrough time                 | Glove thickness | EU standard | Glove comments        |
|----------------|-----------------------------------|-----------------|-------------|-----------------------|
| Natural rubber | See manufacturers recommendations | -               | EN 374      | (minimum requirement) |
| Butyl rubber   |                                   |                 |             |                       |
| Nitrile rubber |                                   |                 |             |                       |
| Neoprene       |                                   |                 |             |                       |
| 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** No protective equipment is needed under normal use conditions.

**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

**Small scale/Laboratory use** Maintain adequate ventilation

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

**Environmental exposure controls** No information available.

## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

|                                                |                          |                                          |
|------------------------------------------------|--------------------------|------------------------------------------|
| <b>Appearance</b>                              | Colorless                |                                          |
| <b>Physical State</b>                          | Liquid                   |                                          |
| <b>Odor</b>                                    | Odorless                 |                                          |
| <b>Odor Threshold</b>                          | No data available        |                                          |
| <b>pH</b>                                      | No information available |                                          |
| <b>Melting Point/Range</b>                     | No data available        |                                          |
| <b>Softening Point</b>                         | No data available        |                                          |
| <b>Boiling Point/Range</b>                     | 121 °C / 249.8 °F        | @ 10 mmHg                                |
| <b>Flash Point</b>                             | No information available | <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>           |                                          |
| Hexanoic acid, 3,5,5-trimethyl-                | 3.2                      |                                          |

## 3,5,5-Trimethylhexanoic acid

|                                  |                          |
|----------------------------------|--------------------------|
| <b>Autoignition Temperature</b>  | No data available        |
| <b>Decomposition Temperature</b> | No data available        |
| <b>Viscosity</b>                 | No data available        |
| <b>Explosive Properties</b>      | No information available |
| <b>Oxidizing Properties</b>      | No information available |

|                          |           |
|--------------------------|-----------|
| <b>Molecular Formula</b> | C9 H18 O2 |
| <b>Molecular Weight</b>  | 158.24    |

## SECTION 10. STABILITY AND REACTIVITY

|                                 |                                 |
|---------------------------------|---------------------------------|
| <b>Stability</b>                | Stable under normal conditions. |
| <b>Hazardous Reactions</b>      | No information available.       |
| <b>Hazardous Polymerization</b> | No information available.       |
| <b>Conditions to Avoid</b>      | Incompatible products.          |
| <b>Materials to avoid</b>       | Strong oxidizing agents.        |

**Hazardous Decomposition Products** Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11. TOXICOLOGICAL INFORMATION

## Product Information

## (a) acute toxicity;

| Component                       | LD50 Oral                 | LD50 Dermal               | LC50 Inhalation |
|---------------------------------|---------------------------|---------------------------|-----------------|
| Hexanoic acid, 3,5,5-trimethyl- | LD50 = 1100 mg/kg ( Rat ) | LD50 > 2000 mg/kg ( Rat ) |                 |

(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 |

(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; Category 3

**Results / Target organs** Respiratory system

(i) STOT-repeated exposure; No data available

**Target Organs** No information available.

# SAFETY DATA SHEET

## 3,5,5-Trimethylhexanoic acid

(j) aspiration hazard; No data available

**Other Adverse Effects** The toxicological properties have not been fully investigated.

**Symptoms / effects, both acute and delayed** No information available

### SECTION 12. ECOLOGICAL INFORMATION

**Ecotoxicity effects** .

**Persistence and Degradability Persistence** No information available  
Persistence is unlikely.

**Bioaccumulative Potential** Bioaccumulation is unlikely

| Component                       | log Pow | Bioconcentration factor (BCF) |
|---------------------------------|---------|-------------------------------|
| Hexanoic acid, 3,5,5-trimethyl- | 3.2     | No data available             |

**Mobility in soil**

**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.

**Other Information** 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**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan

**3,5,5-Trimethylhexanoic acid**

(ISHL), Australia (AICS), Korea (KECL).

| 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     |
|---------------------------------|-----------------------------------------------------|-----------------------------------------|------|-------|-----------|------|-----|-------|------|------|------|----------|
| Hexanoic acid, 3,5,5-trimethyl- | -                                                   | -                                       | X    | X     | 221-975-0 | X    | X   | X     | X    | X    | X    | KE-34559 |

**National Regulations****SECTION 16. OTHER INFORMATION**

**Prepared By** Health, Safety and Environmental Department  
**Revision Date** 12-Sep-2025  
**Revision Summary** Not applicable.

**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/NDL** - 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

**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**

**SAFETY DATA SHEET**

3,5,5-Trimethylhexanoic acid

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The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**