

ALFAAL13360

3,5,5-Trimethylhexanoic acid

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

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

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

Supplier Alfa Aesar
 Avocado Research Chemicals, Ltd.
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 www.alfa.com
 Product Safety Department

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



3,5,5-Trimethylhexanoic acid

Signal Word

Warning

Hazard Statements

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. .

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
Hexanoic acid, 3,5,5-trimethyl-	3302-10-1	95

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

Treat symptomatically.

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

Water spray. Carbon dioxide (CO₂). 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

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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 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	-	EN 374	(minimum requirement)
Butyl rubber	recommendations			
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

Appearance	Colorless	
Physical State	Liquid	
Odor	Odorless	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	121 °C / 249.8 °F	@ 10 mmHg
Flash Point	No information available	Method - No information available
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Vapor Pressure	No data available	
Vapor Density	No data available	(Air = 1.0)
Specific Gravity / Density	No data available	
Bulk Density	Not applicable	Liquid
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	

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Hexanoic acid, 3,5,5-trimethyl-	3.2
Autoignition Temperature	No data available
Decomposition Temperature	No data available
Viscosity	No data available
Explosive Properties	No information available
Oxidizing Properties	No information available

Molecular Formula	C9 H18 O2
Molecular Weight	158.24

SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under normal conditions.
Hazardous Reactions	No information available.
Hazardous Polymerization	No information available.
Conditions to Avoid	Incompatible products.
Materials to avoid	Strong oxidizing agents.

Hazardous Decomposition Products Carbon monoxide (CO). Carbon dioxide (CO₂).

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;

Respiratory	No data available
Skin	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
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(i) STOT-repeated exposure; No data available

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Target Organs No information available.

(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 No information available
Persistence 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

SAFETY DATA SHEET**3,5,5-Trimethylhexanoic acid**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (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 22-Jan-2021
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/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

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 Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

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

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