

ALFAAB24247

3,4,5-Trimethoxyphenylacetonitrile

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

产品说明: Product Description:	3,4,5-三甲氧基苯乙腈 3,4,5-Trimethoxyphenylacetonitrile
Cat No. :	B24247
Synonyms	3,4,5-Trimethoxybenzyl cyanide
CAS No	13338-63-1
Molecular Formula	C11 H13 N O3
Supplier	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
Emergency Telephone Number	For information US call: 001-800-227-6701 / Europe call: +32 14 57 52 11 Emergency Number US :001-201-796-7100 / Europe : +32 14 57 52 99 CHEMTREC Tel. No. US :001-800-424-9300 / Europe :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

Physical State Powder Solid	Appearance Beige	Odor Odorless
Emergency Overview Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation.		

Classification of the substance or mixture

Acute Oral Toxicity	Category 4
Acute Dermal Toxicity	Category 4
Acute Inhalation Toxicity - Dusts and Mists	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3

Label Elements

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

H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation
H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

Precautionary Statements**Prevention**

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P271 - Use only outdoors or in a well-ventilated area
P264 - Wash face, hands and any exposed skin thoroughly after handling
P270 - Do not eat, drink or smoke when using this product
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
P330 - Rinse mouth
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

Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation.

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil.

This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
3,4,5-Trimethoxyphenylacetonitrile	13338-63-1	97

SECTION 4. FIRST AID MEASURES**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 soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.

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Inhalation

Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.

Ingestion

Clean mouth with water. Get medical attention.

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. Chemical 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.

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

Sweep up and shovel into suitable containers for disposal. Do not let this chemical enter the environment.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE

Handling

Avoid contact with skin and eyes. Do not breathe dust. Do not ingest. If swallowed then seek immediate medical assistance.

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

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3,4,5-Trimethoxyphenylacetone nitrile

Control Parameters

Component	China	Taiwan	Thailand	Hong Kong
3,4,5-Trimethoxyphenylacetone nitrile	-	TWA: 5 mg/m ³		Ceiling: 5 mg/m ³

Component	ACGIH TLV	OSHA PEL	NIOSH	The United Kingdom	European Union
3,4,5-Trimethoxyphenylacetone nitrile		(Vacated) TWA: 5 mg/m ³	IDLH: 25 mg/m ³	STEL: 15 mg/m ³ 15 min TWA: 5 mg/m ³ 8 hr Skin	

Legend

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

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. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

Exposure Controls

Engineering Measures

Ensure adequate ventilation, especially in confined areas. 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.

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 Neoprene Natural rubber PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

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 Wear appropriate protective gloves and clothing to prevent skin exposure

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: Particulates filter conforming to EN 143

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:- Particle filtering: EN149:2001

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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 No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	Beige	
Physical State	Powder Solid	
Odor	Odorless	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	76 - 79 °C / 168.8 - 174.2 °F	
Softening Point	No data available	
Boiling Point/Range	No information available	
Flash Point	No information available	Method - No information available
Evaporation Rate	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Vapor Pressure	No data available	
Vapor Density	Not applicable	Solid
Specific Gravity / Density	No data available	
Bulk Density	No data available	
Water Solubility	Insoluble	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	Not applicable	Solid
Explosive Properties	No information available	
Oxidizing Properties	No information available	
Molecular Formula	C11 H13 N O3	
Molecular Weight	207.23	

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. Strong acids. Strong bases.
Hazardous Decomposition Products	Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO ₂). Hydrogen cyanide (hydrocyanic acid).

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

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(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
(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	Not applicable
	Solid
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	Do not empty into drains.
Persistence and Degradability	
Persistence	Insoluble in water.
Bioaccumulative Potential	May have some potential to bioaccumulate
Mobility in soil	Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water solubility
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

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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**

UN-No UN3439
Proper Shipping Name NITRILES, SOLID, TOXIC, N.O.S.
Hazard Class 6.1
Packing Group III

IMDG/IMO

UN-No UN3439
Proper Shipping Name NITRILES, SOLID, TOXIC, N.O.S.
Hazard Class 6.1
Packing Group III

IATA

UN-No UN3439
Proper Shipping Name NITRILES, SOLID, TOXIC, N.O.S.
Hazard Class 6.1
Packing Group III

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/NDL), 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
3,4,5-Trimethoxyphenylacetonitrile	-	-	X	-	236-388-5	-	-	-	-		-	-

National Regulations**SECTION 16. OTHER INFORMATION**

Prepared By
Revision Date

Health, Safety and Environmental Department
27-Apr-2024

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Revision Summary

New emergency telephone response service provider.

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

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

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