

SAFETY DATA SHEET

Revision Date 24-December-2021

Revision Number 4

1. Identification

Product Name 3,4,5-Trimethoxyphenylacetone nitrile

Cat No. : AC151060000; AC151060050; AC151060100; AC151061000

CAS-No 13338-63-1

Synonyms 3,4,5-Trimethoxybenzyl cyanide

Recommended Use Laboratory chemicals.

Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Importer/Distributor

Fisher Scientific
112 Colonnade Road,
Ottawa, ON K2E 7L6,
Canada
Tel: 1-800-234-7437

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Manufacturer

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Emergency Telephone Number For information **US** call: 001-800-ACROS-01 / **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

2. Hazard(s) identification

Classification

WHMIS 2015 Classification Classified as hazardous under the Hazardous Products Regulations (SOR/2015-17)

Acute oral toxicity	Category 4
Acute dermal toxicity	Category 4
Acute Inhalation Toxicity	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

Label Elements

Signal Word

Warning

Hazard Statements

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

**Precautionary Statements****Prevention**

Avoid breathing dust/fume/gas/mist/vapors/spray
Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Use only outdoors or in a well-ventilated area
Wear protective gloves/protective clothing/eye protection/face protection

Response

IF ON SKIN: Wash with plenty of soap and water
IF INHALED: Remove person to fresh air and keep comfortable for breathing
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
Call a POISON CENTER/ doctor if you feel unwell
Rinse mouth
Take off contaminated clothing

Storage

Store in a well-ventilated place. Keep container tightly closed
Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

3. Composition/Information on Ingredients

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

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.
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/effects	No information available.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam.

Unsuitable Extinguishing Media No information available

Flash Point No information available
Method - No information available

Autoignition Temperature No information available

Explosion Limits

Upper No data available

Lower No data available

Sensitivity to Mechanical Impact No information available

Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Nitrogen oxides (NO_x). Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen cyanide (hydrocyanic acid).

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.

NFPA

Health
2

Flammability
1

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions Ensure adequate ventilation. Use personal protective equipment as required.

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.

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. Incompatible Materials. Strong oxidizing agents. Strong acids. Strong bases.

8. Exposure controls / personal protection

Exposure Guidelines

Component	Alberta	British Columbia	Ontario TWAEV	Quebec	ACGIH TLV	OSHA PEL	NIOSH IDLH
3,4,5-Trimethoxyphenyl acetonitrile				Ceiling: 10 ppm Ceiling: 11 mg/m ³ Skin		(Vacated) TWA: 5 mg/m ³	IDLH: 25 mg/m ³

Legend

OSHA - Occupational Safety and Health Administration

NIOSH IDLH: NIOSH - National Institute for Occupational Safety and Health

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

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	Glove comments
Nitrile rubber	See manufacturers	-	Splash protection only
Neoprene	recommendations		
Natural rubber			
PVC			

Inspect gloves before use. observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information) gloves are suitable for the task: Chemical compatability, 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. gloves with care avoiding skin contamination.

Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Recommended Filter type: Particulates filter conforming to EN 143

When RPE is used a face piece Fit Test should be conducted

Environmental exposure controls

No information available.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

9. Physical and chemical properties

Physical State	Powder Solid
Appearance	Beige
Odor	Odorless
Odor Threshold	No information available
pH	No information available
Melting Point/Range	76 - 79 °C / 168.8 - 174.2 °F
Boiling Point/Range	No information available
Flash Point	No information available
Evaporation Rate	Not applicable
Flammability (solid,gas)	No information available
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	Not applicable
Specific Gravity	No information available
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	Not applicable
Molecular Formula	C11 H13 N O3

Molecular Weight

207.23

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Incompatible products.
Incompatible Materials	Strong oxidizing agents, Strong acids, Strong bases
Hazardous Decomposition Products	Nitrogen oxides (NO _x), Carbon monoxide (CO), Carbon dioxide (CO ₂), Hydrogen cyanide (hydrocyanic acid)
Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Component Information

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	No information available
Sensitization	No information available
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
3,4,5-Trimethoxyphenylacetonitrile	13338-63-1	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Respiratory system

STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects, both acute and delayed No information available

Endocrine Disruptor Information No information available

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

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability	Insoluble in water
Bioaccumulation/ Accumulation	No information available.
Mobility	Is not likely mobile in the environment due its low water solubility.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

UN-No	UN3439
Hazard Class	6.1
Packing Group	III

TDG

UN-No	UN3439
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

IMDG/IMO

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

15. Regulatory information

International Inventories

Component	CAS-No	DSL	NDSL	TSCA	TSCA Inventory notification - Active-Inactive	EINECS	ELINCS	NLP
3,4,5-Trimethoxyphenylacetonitrile	13338-63-1	-	-	-	-	236-388-5	-	-

Component	CAS-No	IECSC	KECL	ENCS	ISHL	TCSI	AICS	NZIoC	PICCS
3,4,5-Trimethoxyphenylacetonitrile	13338-63-1	-	-	-	-	X	-	-	-

Legend:

X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

Canada

SDS in compliance with provisions of information as set out in Canadian Standard - Part 4, Schedule 1 and 2 of the Hazardous Products Regulations (HPR) and meets the requirements of the HPR (Paragraph 13(1)(a) of the Hazardous Products Act (HPA)).

Component	Canada - National Pollutant Release Inventory (NPRI)	Canadian Environmental Protection Agency (CEPA) - List of Toxic Substances	Canada's Chemicals Management Plan (CEPA)
3,4,5-Trimethoxyphenylacetonitrile	Part 1, Group A Substance		

Other International Regulations**Authorisation/Restrictions according to EU REACH****Safety, health and environmental regulations/legislation specific for the substance or mixture**

Component	CAS-No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
3,4,5-Trimethoxyphenylacetonitrile	13338-63-1	Not applicable	Not applicable	Not applicable	Not applicable

Component	CAS-No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
3,4,5-Trimethoxyphenylacetonitrile	13338-63-1	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By Regulatory Affairs
Thermo Fisher Scientific
Email: EMSDS.RA@thermofisher.com

Revision Date 24-December-2021

Print Date 24-December-2021

Revision Summary This document has been updated to comply with the requirements of WHMIS 2015 to align with the Globally Harmonised System (GHS) for the Classification and Labelling of Chemicals.

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 SDS