

SAFETY DATA SHEET

Revision Date 24-Dec-2021

Revision Number 4

1. Identification

Product Name 3,4,5-Trimethoxyphenylacetonitrile

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

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

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

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

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

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
Target Organs - Respiratory system.	

Label Elements**Signal Word**

Warning

Hazard Statements

Causes skin irritation

Causes serious eye irritation

May cause respiratory irritation

Harmful if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling

Do not eat, drink or smoke when using this product

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

Avoid breathing dust/fume/gas/mist/vapors/spray

Use only outdoors or in a well-ventilated area

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

Call a POISON CENTER or doctor/physician if you feel unwell

Skin

IF ON SKIN: Wash with plenty of soap and water

Call a POISON CENTER or doctor/physician if you feel unwell

If skin irritation occurs: Get medical advice/attention

Take off contaminated clothing and wash before reuse

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

If eye irritation persists: Get medical advice/attention

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell

Rinse mouth

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

Hazards not otherwise classified (HNOC)

None identified

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 and effects	No information available.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray. Carbon dioxide (CO ₂). 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	Flammability	Instability	Physical hazards
2	1	0	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	ACGIH TLV	OSHA PEL	NIOSH IDLH	Mexico OEL (TWA)
3,4,5-Trimethoxyphenylacet onitrile		(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.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection 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.

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

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 (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂), 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

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
3,4,5-Trimethoxyphenylacetonitrile	13338-63-1	-	-	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
3,4,5-Trimethoxyphenylacetonitrile	13338-63-1	-	-	236-388-5	-	-	-	-	-	-

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

U.S. Federal Regulations**SARA 313**

Component	CAS No	Weight %	SARA 313 - Threshold Values %
3,4,5-Trimethoxyphenylacetonitrile	13338-63-1	97	1.0

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act)

Not applicable

Component	CWA - Hazardous Substances	CWA - Reportable Quantities	CWA - Toxic Pollutants	CWA - Priority Pollutants
3,4,5-Trimethoxyphenylacetonitrile	-	-	X	X

Clean Air Act

Not applicable

Component	HAPS Data	Class 1 Ozone Depletors	Class 2 Ozone Depletors
3,4,5-Trimethoxyphenylacetone nitrile	X		-

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA Not applicable

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
3,4,5-Trimethoxyphenylacetone nitrile	-	X	X	X	X

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant Y
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

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-Trimethoxyphenylacetone nitrile	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-Trimethoxyphenylacetone nitrile	13338-63-1	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

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Revision Summary This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

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