

SAFETY DATA SHEET

Revision Date 14-Feb-2020

Revision Number 2

1. Identification

Product Name 3,4,5-Trimethoxyphenylacetonitrile

Cat No. : B24247

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

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Emergency Telephone Number

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660.
After normal business hours, call Carechem 24 at (866) 928-0789.

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 (CO₂). Dry chemical. Chemical foam.

Unsuitable Extinguishing Media No information available

Flash Point No information available
Method - No information available

Autoignition Temperature

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. Refer product specification and/or product label for specific storage temperature requirement. Keep container tightly closed.

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	
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 (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

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

X - Listed

'-' - Not Listed

TSCA 12(b) - Notices of Export Not applicable

International Inventories

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

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

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-Trimethoxyphenylacetonitrile	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-Trimethoxyphenylacetonitrile	-	X	X	X	X

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant N
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

16. Other information

Prepared By Health, Safety and Environmental Department
Email: tech@alfa.com
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Revision Summary SDS authoring systems update, replaces ChemGes SDS No. 13338-63-1.

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