

1 Identification

Product identifier

Product name: 1,3-Phenylenediacetonitrile

Stock number: A15323, L02851

CAS Number:

626-22-2

EC number:

210-936-3

Relevant identified uses of the substance or mixture and uses advised against.

Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet

Manufacturer/Supplier:

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

Information Department: Health, Safety and Environmental Department

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 of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)



GHS06 Skull and crossbones

Acute Tox. 3 H301 Toxic if swallowed.

Acute Tox. 3 H311 Toxic in contact with skin.

Acute Tox. 3 H331 Toxic if inhaled.

Hazards not otherwise classified No information known.

Label elements

GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms



GHS06

Signal word

Danger

Hazard statements

H301+H311+H331 Toxic if swallowed, in contact with skin or if inhaled.

Precautionary statements

P280 Wear protective gloves / protective clothing.

P309 IF exposed or if you feel unwell:

P310 Immediately call a POISON CENTER/doctor/...

WHMIS classification

D1A - Very toxic material causing immediate and serious toxic effects



Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH 2 Health (acute effects) = 2

FIRE 1 Flammability = 1

REACTIVITY 1 Physical Hazard = 1

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances

CAS# Description:

626-22-2 1,3-Phenylenediacetonitrile

Identification number(s):

EC number: 210-936-3

4 First-aid measures

Description of first aid measures

General information

Immediately remove any clothing soiled by the product.

Remove breathing apparatus only after contaminated clothing has been completely removed.

In case of irregular breathing or respiratory arrest provide artificial respiration.

After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm.

Seek immediate medical advice.

After skin contact

Immediately wash with water and soap and rinse thoroughly.

Seek immediate medical advice.

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After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.

After swallowing Do not induce vomiting; immediately call for medical help.

Information for doctor

Most important symptoms and effects, both acute and delayed No further relevant information available.

Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures

Extinguishing media

Suitable extinguishing agents Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Special hazards arising from the substance or mixture

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

Nitrogen oxides (NO_x)

Hydrogen cyanide (HCN)

Advice for firefighters

Protective equipment:

Wear self-contained respirator.

Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

Environmental precautions: Do not allow material to be released to the environment without proper governmental permits.

Methods and material for containment and cleaning up:

Dispose of contaminated material as waste according to section 13.

Ensure adequate ventilation.

Prevention of secondary hazards: No special measures required.

Reference to other sections

See Section 7 for information on safe handling

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

7 Handling and storage

Handling

Precautions for safe handling

Keep container tightly sealed.

Store in cool, dry place in tightly closed containers.

Ensure good ventilation at the workplace.

Open and handle container with care.

Information about protection against explosions and fires: No information known.

Conditions for safe storage, including any incompatibilities

Storage

Requirements to be met by storerooms and receptacles: No special requirements.

Information about storage in one common storage facility:

Store away from oxidizing agents.

Store away from strong bases.

Further information about storage conditions:

Keep container tightly sealed.

Store in cool, dry conditions in well sealed containers.

Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Control parameters

Components with limit values that require monitoring at the workplace:

626-22-2 1,3-Phenylenediacetonitrile (100.0%)

PEL (USA)	Long-term value: 5 mg/m ³ as CN; Skin
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Additional information: No data

Exposure controls

Personal protective equipment

General protective and hygienic measures

The usual precautionary measures for handling chemicals should be followed.

Keep away from foodstuffs, beverages and feed.

Remove all soiled and contaminated clothing immediately.

Wash hands before breaks and at the end of work.

Store protective clothing separately.

Avoid contact with the eyes and skin.

Maintain an ergonomically appropriate working environment.

Breathing equipment: Use self-contained respiratory protective device in emergency situations.

Protection of hands:

Impervious gloves

Check protective gloves prior to each use for their proper condition.

The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.

Penetration time of glove material (in minutes) Not determined

Eye protection: Safety glasses

Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties

General Information

Appearance:

Form: Crystalline

Color: Off-white

Odor: Not determined

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Odor threshold:	Not determined.
pH-value:	Not applicable.
Change in condition	
Melting point/Melting range:	32-35 °C (90-95 °F)
Boiling point/Boiling range:	169-171 °C (336-340 °F) (25 mmHg)
Sublimation temperature / start:	Not determined
Flash point:	> 110 °C (> 230 °F)
Flammability (solid, gaseous)	Not determined.
Ignition temperature:	Not determined
Decomposition temperature:	Not determined
Auto igniting:	Not determined.
Danger of explosion:	Product does not present an explosion hazard.
Explosion limits:	
Lower:	Not determined
Upper:	Not determined
Vapor pressure:	Not applicable.
Density:	Not determined
Relative density	Not determined.
Vapor density	Not applicable.
Evaporation rate	Not applicable.
Solubility in / Miscibility with	
Water:	Insoluble
Partition coefficient (n-octanol/water):	Not determined.
Viscosity:	
dynamic:	Not applicable.
kinematic:	Not applicable.
Other information	No further relevant information available.

10 Stability and reactivity

Reactivity No information known.
Chemical stability Stable under recommended storage conditions.
Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.
Possibility of hazardous reactions No dangerous reactions known
Conditions to avoid No further relevant information available.
Incompatible materials:
Oxidizing agents
Bases
Hazardous decomposition products:
Carbon monoxide and carbon dioxide
Nitrogen oxides
Hydrogen cyanide

11 Toxicological information

Information on toxicological effects
Acute toxicity:
Toxic in contact with skin.
Toxic if inhaled.
Toxic if swallowed.
Danger through skin absorption.
LD/LC50 values that are relevant for classification: No data
Skin irritation or corrosion: May cause irritation
Eye irritation or corrosion: May cause irritation
Sensitization: No sensitizing effects known.
Germ cell mutagenicity: No effects known.
Carcinogenicity: No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.
Reproductive toxicity: No effects known.
Specific target organ system toxicity - repeated exposure: No effects known.
Specific target organ system toxicity - single exposure: No effects known.
Aspiration hazard: No effects known.
Subacute to chronic toxicity: No effects known.
Subacute to chronic toxicity:
Nitriles may resemble cyanides in toxicity. Exposure to nitriles may cause increased salivation, flushing of the face, eye and respiratory tract irritation, shallow respiration, nausea, vomiting, weakness, headache and diarrhea. Jaundice, anemia, and leucocytosis has been reported in some cases.
Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

Toxicity
Aquatic toxicity: No further relevant information available.
Persistence and degradability No further relevant information available.
Bioaccumulative potential No further relevant information available.
Mobility in soil No further relevant information available.
Additional ecological information:
General notes:
Do not allow material to be released to the environment without proper governmental permits.
Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.
Avoid transfer into the environment.
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.
Other adverse effects No further relevant information available.

13 Disposal considerations

Waste treatment methods
Recommendation Consult state, local or national regulations to ensure proper disposal.

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USA

Product name: 1,3-Phenylenediacetonitrile**Uncleaned packagings:****Recommendation:** Disposal must be made according to official regulations.

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14 Transport information**UN-Number**
DOT, IMDG, IATA

UN3439

UN proper shipping name
DOT
IMDG, IATANitriles, solid, toxic, n.o.s. (1,3-Phenylenediacetonitrile)
NITRILES, SOLID, TOXIC, N.O.S. (1,3-Phenylenediacetonitrile)**Transport hazard class(es)**
DOT**Class**
Label
Class
Label
IMDG, IATA6.1 Toxic substances.
6.1
6.1 (T2) Toxic substances
6.1**Class**
Label6.1 Toxic substances.
6.1**Packing group**
DOT, IMDG, IATA

III

Environmental hazards:

Not applicable.

Special precautions for user

Warning: Toxic substances

Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code Not applicable.**Transport/Additional information:****DOT**
Marine Pollutant (DOT):

No

UN "Model Regulation":

UN3439, Nitriles, solid, toxic, n.o.s. (1,3-Phenylenediacetonitrile), 6.1, III

15 Regulatory information**Safety, health and environmental regulations/legislation specific for the substance or mixture****GHS label elements** The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)**Hazard pictograms**

GHS06

Signal word Danger**Hazard statements**

H301+H311+H331 Toxic if swallowed, in contact with skin or if inhaled.

Precautionary statements

P280 Wear protective gloves / protective clothing.

P309 IF exposed or if you feel unwell:

P310 Immediately call a POISON CENTER/doctor/...

National regulations

This product is not listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical Substance Inventory. Use of this product is restricted to research and development only. This product must be used by or directly under the supervision of a technically qualified individual as defined by TSCA. This product must not be used for commercial purposes or in formulations for commercial purposes.

SARA Section 313 (specific toxic chemical listings) Substance is not listed.**California Proposition 65****Prop 65 - Chemicals known to cause cancer** Substance is not listed.**Prop 65 - Developmental toxicity** Substance is not listed.**Prop 65 - Developmental toxicity, female** Substance is not listed.**Prop 65 - Developmental toxicity, male** Substance is not listed.**Information about limitation of use:** For use only by technically qualified individuals.**Other regulations, limitations and prohibitive regulations****Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006.** Substance is not listed.**The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.**

Substance is not listed.

Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.**Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.**16 Other information**

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department**Date of preparation / last revision** 11/23/2015 / -**Abbreviations and acronyms:**

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)

IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)

ICAO: International Civil Aviation Organization

ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

EINECS: European Inventory of Existing Commercial Chemical Substances

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USA

Product name: 1,3-Phenylenediacetonitrile

CAS: Chemical Abstracts Service (division of the American Chemical Society)
HMIS: Hazardous Materials Identification System (USA)
WHMIS: Workplace Hazardous Materials Information System (Canada)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
vPvB: very Persistent and very Bioaccumulative
ACGIH: American Conference of Governmental Industrial Hygienists (USA)
OSHA: Occupational Safety and Health Administration (USA)
NTP: National Toxicology Program (USA)
IARC: International Agency for Research on Cancer
EPA: Environmental Protection Agency (USA)

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