

SAFETY DATA SHEET

Creation Date 01-May-2012

Revision Date 24-Dec-2021

Revision Number 5

1. Identification

Product Name 1,4-Dicyanobutane

Cat No. : AC113830000; AC113830010; AC113830050; AC113831000;
AC113832500

CAS No 111-69-3
Synonyms Adiponitrile

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
Acute Inhalation Toxicity - Vapors

Category 3
Category 4

Label Elements

Signal Word
Danger

Hazard Statements
Toxic if swallowed
Harmful 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

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

Ingestion

IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician

Rinse mouth

Storage

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 %
Adiponitrile	111-69-3	>95

4. First-aid measures

General Advice	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
Ingestion	Do NOT induce vomiting. Call a physician or poison control center immediately.
Most important symptoms and effects	None reasonably foreseeable.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam.

Unsuitable Extinguishing Media No information available

Flash Point 163 °C / 325.4 °F

Method - No information available

Autoignition Temperature 500 °C / 932 °F

Explosion Limits

Upper 4.99%

Lower 1.70%

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. Thermal decomposition can lead to release of irritating gases and vapors.

NFPA

Health
3

Flammability
1

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions

Ensure adequate ventilation. Use personal protective equipment as required. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas.

Environmental Precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up Keep in suitable, closed containers for disposal. Soak up with inert absorbent material.

7. Handling and storage

Handling

Do not get in eyes, on skin, or on clothing. Wear personal protective equipment/face protection. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Use only under a chemical fume hood.

Storage.

Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Incompatible Materials. Strong oxidizing agents. Strong acids. Strong bases. Strong reducing agents.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH	Mexico OEL (TWA)
Adiponitrile	TWA: 2 ppm Skin	(Vacated) TWA: 5 mg/m ³	IDLH: 25 mg/m ³ TWA: 4 ppm TWA: 18 mg/m ³	TWA: 2 ppm

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

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

Engineering Measures Use explosion-proof electrical/ventilating/lighting equipment. 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	Liquid
Appearance	Light yellow
Odor	Odorless
Odor Threshold	No information available
pH	No information available
Melting Point/Range	1 - 3 °C / 33.8 - 37.4 °F
Boiling Point/Range	295 °C / 563 °F @ 760 mmHg
Flash Point	163 °C / 325.4 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	4.99%
Lower	1.70%
Vapor Pressure	2.5 hPa @ 119 °C
Vapor Density	3.7
Specific Gravity	0.950
Solubility	Soluble in water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	500 °C / 932 °F
Decomposition Temperature	No information available
Viscosity	5.8 cp at 30 °C
Molecular Formula	C6 H8 N2
Molecular Weight	108.14

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, Strong reducing agents
Hazardous Decomposition Products	Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO ₂), Hydrogen cyanide (hydrocyanic acid)
Hazardous Polymerization	Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Adiponitrile	LD50 = 138 mg/kg (Rat)	LD50 = 2134 mg/kg (Rabbit)	LC50 = 2.9 mg/l (Rat) 4 h

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
Adiponitrile	111-69-3	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 None known

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. .

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Adiponitrile	Not listed	LC50: = 775 mg/L, 96h (Poecilia reticulata) LC50: = 820 mg/L, 96h static (Pimephales promelas) LC50: 1850 - 2020 mg/L, 96h flow-through (Pimephales promelas) LC50: = 720 mg/L, 96h static (Lepomis macrochirus)	EC50 = 393 mg/L 5 min EC50 = 402 mg/L 15 min EC50 = 411 mg/L 30 min	EC50: > 1000 mg/L, 48h (Daphnia magna)

Persistence and Degradability Persistence is unlikely

Bioaccumulation/ Accumulation No information available.

Mobility . Will likely be mobile in the environment due to its water solubility.

Component	log Pow
Adiponitrile	-0.32

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 UN2205
 Proper Shipping Name ADIPONITRILE
 Hazard Class 6.1
 Packing Group III

TDG

UN-No UN2205
 Proper Shipping Name ADIPONITRILE
 Hazard Class 6.1
 Packing Group III

IATA

UN-No UN2205
 Proper Shipping Name ADIPONITRILE
 Hazard Class 6.1
 Packing Group III

IMDG/IMO

UN-No UN2205
 Proper Shipping Name ADIPONITRILE
 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
Adiponitrile	111-69-3	X	ACTIVE	-

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
Adiponitrile	111-69-3	X	-	203-896-3	X	X	X	X	X	KE-00274

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
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			Values %
Adiponitrile	111-69-3	>95	1.0

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

CWA (Clean Water Act)

Component	CWA - Hazardous Substances	CWA - Reportable Quantities	CWA - Toxic Pollutants	CWA - Priority Pollutants
Adiponitrile	-	-	X	X

Clean Air Act

Component	HAPS Data	Class 1 Ozone Depleters	Class 2 Ozone Depleters
Adiponitrile	X		-

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA This material, as supplied, contains one or more substances regulated as a hazardous substance under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302)

Component	Hazardous Substances RQs	CERCLA EHS RQs
Adiponitrile	-	1000 lb

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
Adiponitrile	X	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)
Adiponitrile	111-69-3	Listed	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)
Adiponitrile	111-69-3	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By	Regulatory Affairs Thermo Fisher Scientific Email: EMSDS.RA@thermofisher.com
Creation Date	01-May-2012
Revision Date	24-Dec-2021
Print Date	24-Dec-2021
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