

# SAFETY DATA SHEET

Version 6.1 Revision Date 04/25/2021 Print Date 02/11/2022

### SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Adiponitrile, >99%, acid < 200 ppm, H2O<

100 ppm

Product Number : 900020 Brand : Aldrich CAS-No. : 111-69-3

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.

3050 SPRUCE ST ST. LOUIS MO 63103 UNITED STATES

Telephone : +1 314 771-5765 Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-

527-3887 CHEMTREC (International) 24

Hours/day; 7 Days/week

#### **SECTION 2: Hazards identification**

#### 2.1 Classification of the substance or mixture

## GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 3), H301 Acute toxicity, Inhalation (Category 4), H332

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)

H301 Toxic if swallowed.

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H332 Harmful if inhaled.

Precautionary statement(s)

P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P271 Use only outdoors or in a well-ventilated area.

P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.

Rinse mouth.

P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable

for breathing. Call a POISON CENTER/ doctor if you feel unwell.

P405 Store locked up.

P501 Dispose of contents/ container to an approved waste disposal

plant.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## **SECTION 3: Composition/information on ingredients**

#### 3.1 Substances

Synonyms : 1,4-Dicyanobutane

Formula : C6H8N2

Molecular weight : 108.14 g/mol

CAS-No. : 111-69-3

EC-No. : 203-896-3

Component	Classification	Concentration
adipic acid dinitrile		
	Acute Tox. 3; Acute Tox. 4; H301, H332	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

### **SECTION 4: First aid measures**

## 4.1 Description of first-aid measures

### **General advice**

Move out of dangerous area. Consult a physician. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.



#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

## 4.3 Indication of any immediate medical attention and special treatment needed

No data available

## **SECTION 5: Firefighting measures**

## 5.1 Extinguishing media

### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NOx)

Hydrogen cyanide (hydrocyanic acid)

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### 5.4 Further information

No data available

#### **SECTION 6: Accidental release measures**

## 6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

#### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

#### 6.4 Reference to other sections

For disposal see section 13.

## **SECTION 7: Handling and storage**

#### 7.1 Precautions for safe handling

## Advice on safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

#### **Hygiene measures**

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

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For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

### Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

strongly hygroscopic Handle and store under inert gas.

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

## 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

## **SECTION 8: Exposure controls/personal protection**

### 8.1 Control parameters

Ingredients with workplace control parameters

Ingredients with workplace control parameters					
Component	CAS-No.	Value	Control parameters	Basis	
adipic acid dinitrile	111-69-3	TWA	2 ppm	USA. ACGIH Threshold Limit Values (TLV)	
	Remarks	Danger of cutaneous absorption			
		TWA	4 ppm 18 mg/m3	USA. NIOSH Recommended Exposure Limits	
		PEL	2 ppm 8.8 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)	
		Skin			

## 8.2 Exposure controls

### **Appropriate engineering controls**

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

### Personal protective equipment

### Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

#### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

#### **Body Protection**

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.



#### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a fullface respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

## **SECTION 9: Physical and chemical properties**

### Information on basic physical and chemical properties

a) Appearance Form: liquid

Color: light brown

No data available b) Odor c) Odor Threshold No data available No data available d) pH

e) Melting Melting point/range: 0 - 1 °C (32 - 34 °F)

point/freezing point

161 - 162 °C 322 - 324 °F at 15 hPa Initial boiling point

and boiling range 295 °C (563 °F) at 1013 hPa

g) Flash point > 110 °C (> 230 °F)

h) Evaporation rate No data available Flammability (solid, No data available

gas)

explosive limits

Upper explosion limit: 4.99 %(V) Upper/lower j) Lower explosion limit: 1.7 %(V) flammability or

No data available k) Vapor pressure Vapor density 3.73 - (Air = 1.0)

m) Relative density No data available n) Water solubility No data available

No data available o) Partition coefficient: n-octanol/water

p) Autoignition No data available temperature

No data available q) Decomposition temperature

No data available r) Viscosity No data available s) Explosive properties Oxidizing properties No data available

## 9.2 Other safety information

Relative vapor 3.73 - (Air = 1.0)

# **SECTION 10: Stability and reactivity**

### 10.1 Reactivity

No data available

#### 10.2 Chemical stability

Stable under recommended storage conditions.

#### 10.3 Possibility of hazardous reactions

No data available

#### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Strong oxidizing agentsStrong acids, Strong bases, Strong oxidizing agents, Strong reducing agents

## 10.6 Hazardous decomposition products

In the event of fire: see section 5

### **SECTION 11: Toxicological information**

### 11.1 Information on toxicological effects

### **Acute toxicity**

LD50 Oral - Rat - male and female - 215 mg/kg

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation

Serious eye damage/eye irritation

Respiratory or skin sensitization

No data available

# Germ cell mutagenicity

No data available

## Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is

identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is

identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is

on OSHA's list of regulated carcinogens.

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## Reproductive toxicity

No data available

## Specific target organ toxicity - single exposure

No data available

### Specific target organ toxicity - repeated exposure

No data available

### **Aspiration hazard**

No data available

#### 11.2 Additional Information

Not available

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

## **SECTION 12: Ecological information**

### 12.1 Toxicity

Toxicity to fish LC50 - Pimephales promelas (fathead minnow) - 1,930 mg/l - 96 h

### 12.2 Persistence and degradability

No data available

### 12.3 Bioaccumulative potential

No data available

#### 12.4 Mobility in soil

No data available

#### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

#### 12.6 Other adverse effects

No data available

# **SECTION 13: Disposal considerations**

#### 13.1 Waste treatment methods

## **Product**

Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company.

### Contaminated packaging

Dispose of as unused product.

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### **SECTION 14: Transport information**

DOT (US)

UN number: 2205 Class: 6.1 Packing group: III

Proper shipping name: Adiponitrile

Reportable Quantity (RQ): Poison Inhalation Hazard: No

**IMDG** 

UN number: 2205 Class: 6.1 Packing group: III EMS-No: F-A, S-A

Proper shipping name: ADIPONITRILE

**IATA** 

UN number: 2205 Class: 6.1 Packing group: III

Proper shipping name: Adiponitrile

## **SECTION 15: Regulatory information**

## **SARA 302 Components**

The following components are subject to reporting levels established by SARA Title III, Section 302:

adipic acid dinitrile CAS-No. Revision Date 111-69-3 2008-11-03

### **SARA 313 Components**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

#### SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

## **Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

### **Pennsylvania Right To Know Components**

adipic acid dinitrile CAS-No. Revision Date 111-69-3 2008-11-03

## **SECTION 16: Other information**

#### **Further information**

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