

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product name : Adiponitrile  
  
Product Number : D77001  
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  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA  
  
Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

#### 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

### 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.  
H332 Harmful if inhaled.

Precautionary statement(s)

P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ 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

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### 3. COMPOSITION/INFORMATION ON INGREDIENTS

#### 3.1 Substances

Synonyms	:	1,4-Dicyanobutane
Formula	:	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>
Molecular weight	:	108.14 g/mol
CAS-No.	:	111-69-3
EC-No.	:	203-896-3

#### Hazardous components

Component	Classification	Concentration
<b>Adiponitrile</b>	Acute Tox. 3; Acute Tox. 4; H301, H332	90 - 100 %

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

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### 4. FIRST AID MEASURES

#### 4.1 Description of first aid measures

##### General advice

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

##### 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

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### 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

No data available

#### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### 5.4 Further information

No data available

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## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, 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.

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## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

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

For precautions see section 2.2.

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

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.

Storage class (TRGS 510): 6.1D: Non-combustible, acute toxic Cat.3 / toxic hazardous materials or hazardous materials causing chronic effects

### 7.3 Specific end use(s)

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

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Adiponitrile	111-69-3	TWA	2.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Upper Respiratory Tract irritation Lower Respiratory Tract irritation Danger of cutaneous absorption		
		TWA	2 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Upper Respiratory Tract irritation Lower Respiratory Tract irritation Danger of cutaneous absorption		
		TWA	4.000000 ppm 18.000000 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		PEL	2 ppm 8.8 mg/m <sup>3</sup>	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.

#### Full contact

Material: Chloroprene

Minimum layer thickness: 0.6 mm

Break through time: 480 min

Material tested: Camapren® (KCL 722 / Aldrich Z677493, Size M)

#### Splash contact

Material: Nature latex/chloroprene

Minimum layer thickness: 0.6 mm

Break through time: 60 min

Material tested: Lapren® (KCL 706 / Aldrich Z677558, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### 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 full-face 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.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |                                                 |                                                                     |
|-------------------------------------------------|---------------------------------------------------------------------|
| a) Appearance                                   | Form: liquid<br>Colour: light brown                                 |
| b) Odour                                        | No data available                                                   |
| c) Odour Threshold                              | No data available                                                   |
| d) pH                                           | No data available                                                   |
| e) Melting point/freezing point                 | Melting point/range: 1 - 3 °C (34 - 37 °F) - lit.                   |
| f) Initial boiling point and boiling range      | 295 °C (563 °F) - lit.                                              |
| g) Flash point                                  | 163 °C (325 °F) - closed cup                                        |
| h) Evaporation rate                             | No data available                                                   |
| i) Flammability (solid, gas)                    | No data available                                                   |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 4.99 %(V)<br>Lower explosion limit: 1.7 %(V) |

k) Vapour pressure	No data available
l) Vapour density	3.73 - (Air = 1.0)
m) Relative density	0.951 g/cm <sup>3</sup> at 25 °C (77 °F)
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Auto-ignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

## 9.2 Other safety information

Relative vapour density 3.73 - (Air = 1.0)

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## 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 agents Strong acids, Strong bases, Strong oxidizing agents, Strong reducing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Hydrogen cyanide (hydrocyanic acid)

Other decomposition products - No data available

In the event of fire: see section 5

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## 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

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

No data available

### **Carcinogenicity**

- IARC: No component 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 component 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 identified as a carcinogen or potential carcinogen by OSHA.

### **Reproductive toxicity**

No data available

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

### **Additional Information**

RTECS: AV2625000

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

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## **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

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## **13. DISPOSAL CONSIDERATIONS**

### **13.1 Waste treatment methods**

#### **Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. 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.

#### **Contaminated packaging**

Dispose of as unused product.

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## **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

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**15. REGULATORY INFORMATION**

**SARA 302 Components**

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

	CAS-No.	Revision Date
Adiponitrile	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**

	CAS-No.	Revision Date
Adiponitrile	111-69-3	2008-11-03

	CAS-No.	Revision Date
Adiponitrile	111-69-3	2008-11-03

**Pennsylvania Right To Know Components**

	CAS-No.	Revision Date
Adiponitrile	111-69-3	2008-11-03

	CAS-No.	Revision Date
Adiponitrile	111-69-3	2008-11-03

	CAS-No.	Revision Date
Adiponitrile	111-69-3	2008-11-03

**New Jersey Right To Know Components**

	CAS-No.	Revision Date
Adiponitrile	111-69-3	2008-11-03

	CAS-No.	Revision Date
Adiponitrile	111-69-3	2008-11-03

**California Prop. 65 Components**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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**16. OTHER INFORMATION**

**Full text of H-Statements referred to under sections 2 and 3.**

Acute Tox.	Acute toxicity
H301	Toxic if swallowed.
H332	Harmful if inhaled.

**HMIS Rating**

Health hazard:                      2

Chronic Health Hazard: \*  
Flammability: 1  
Physical Hazard 0

**NFPA Rating**

Health hazard: 1  
Fire Hazard: 1  
Reactivity Hazard: 0

**Further information**

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**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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