

Creation Date 01-May-2012

Revision Date 10-Dec-2020

Revision Number 5

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

Product Description: 1,4-Dicyanobutane
Cat No. : 113830000; 113830010; 113830050; 113831000; 113832500
Synonyms Adiponitrile
CAS-No 111-69-3
EC-No. 203-896-3
Molecular Formula C6 H8 N2
Reach Registration Number 01-2119473986-18

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

Recommended Use Laboratory chemicals.
Sector of use SU3 - Industrial uses: Uses of substances as such or in preparations at industrial sites
Product category PC21 - Laboratory chemicals
Process categories PROC15 - Use as a laboratory reagent
Environmental release category ERC6a - Industrial use resulting in manufacture of another substance (use of intermediates)
Uses advised against No Information available

1.3. Details of the supplier of the safety data sheet

Company **UK entity/business name**
 Fisher Scientific UK
 Bishop Meadow Road, Loughborough,
 Leicestershire LE11 5RG, United Kingdom

EU entity/business name
 Acros Organics BVBA
 Janssen Pharmaceuticaaan 3a
 2440 Geel, Belgium

E-mail address begel.sdsdesk@thermofisher.com

1.4. 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

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - Regulation (EC) No 1272/2008

Physical hazards

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Based on available data, the classification criteria are not met

Health hazards

Acute oral toxicity
Acute Inhalation Toxicity - Vapors

Category 3 (H301)
Category 4 (H332)

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Danger

Hazard Statements

H301 - Toxic if swallowed
H332 - Harmful if inhaled

Precautionary Statements

P264 - Wash face, hands and any exposed skin thoroughly after handling
P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

2.3. Other hazards

Toxic to terrestrial vertebrates

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Component	CAS-No	EC-No.	Weight %	CLP Classification - Regulation (EC) No 1272/2008
Adiponitrile	111-69-3	EEC No. 203-896-3	>95	Acute Tox. 3 (H301) Acute Tox. 4 (H332)

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Full text of Hazard Statements: see section 16

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SECTION 4: FIRST AID MEASURES

4.1. Description of 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.
Ingestion	Do NOT induce vomiting. Call a physician or poison control center immediately.
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.
Self-Protection of the First Aider	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

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

None reasonably foreseeable.

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

Notes to Physician Treat symptomatically.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

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

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

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

Hazardous Combustion Products

Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂), Hydrogen cyanide (hydrocyanic acid).

5.3. Advice 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.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

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

6.2. Environmental precautions

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

6.3. Methods and material for containment and cleaning up

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe 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.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

Keep in a dry, cool and well-ventilated place. Keep container tightly closed.

Technical Rules for Hazardous Substances (TRGS) 510 Storage Class (LGK)
(Germany)

Class 6.1C

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

List source(s): **UK** - EH40/2005 Work Exposure Limits, Third edition. Published 2018.

Component	The United Kingdom	European Union	Ireland
Adiponitrile	STEL: 15 mg/m ³ 15 min TWA: 5 mg/m ³ 8 hr Skin		TWA: 2 ppm 8 hr. STEL: 6 ppm 15 min

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of

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exposure to chemical and biological agents.

Derived No Effect Level (DNEL) No information available

<u>Route of exposure</u>	<u>Acute effects (local)</u>	<u>Acute effects (systemic)</u>	<u>Chronic effects (local)</u>	<u>Chronic effects (systemic)</u>
Oral Dermal Inhalation				

Predicted No Effect Concentration (PNEC) No information available.

8.2. Exposure controls

Engineering Measures

Use explosion-proof electrical/ventilating/lighting/equipment. Ensure that eyewash stations and safety showers are close to the workstation location.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

Eye Protection

Goggles (European standard - EN 166)

Hand Protection

Protective gloves

<u>Glove material</u>	<u>Breakthrough time</u>	<u>Glove thickness</u>	<u>EU standard</u>	<u>Glove comments</u>
Nitrile rubber Neoprene Natural rubber PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

Skin and body protection

Long sleeved clothing

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387

Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

When RPE is used a face piece Fit Test should be conducted

Environmental exposure controls No information available.

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SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Light yellow	
Odor	Odorless	
Odor Threshold	No data available	
Melting Point/Range	1 - 3 °C / 33.8 - 37.4 °F	
Softening Point	No data available	
Boiling Point/Range	295 °C / 563 °F	@ 760 mmHg
Flammability (liquid)	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	Lower 1.7 Upper 4.99	
Flash Point	163 °C / 325.4 °F	Method - No information available
Autoignition Temperature	500 °C / 932 °F	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	5.8 cp at 30 °C	
Water Solubility	90 g/L (20°C)	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Adiponitrile	-0.32	
Vapor Pressure	2.5 hPa @ 119 °C	
Density / Specific Gravity	0.950	
Bulk Density	Not applicable	Liquid
Vapor Density	3.7	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

9.2. Other information

Molecular Formula	C6 H8 N2
Molecular Weight	108.14

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

10.4. Conditions to avoid

Incompatible products.

10.5. Incompatible materials

Strong oxidizing agents. Strong acids. Strong bases. Strong reducing agents.

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10.6. Hazardous decomposition products

Nitrogen oxides (NO_x). Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen cyanide (hydrocyanic acid).

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information

(a) acute toxicity;

Oral

Category 3

Dermal

Based on available data, the classification criteria are not met

Inhalation

Category 4

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

(b) skin corrosion/irritation; Based on available data, the classification criteria are not met

(c) serious eye damage/irritation; Based on available data, the classification criteria are not met

(d) respiratory or skin sensitization;

Respiratory

Based on available data, the classification criteria are not met

Skin

Based on available data, the classification criteria are not met

(e) germ cell mutagenicity;

Based on available data, the classification criteria are not met

(f) carcinogenicity;

Based on available data, the classification criteria are not met

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity;

Based on available data, the classification criteria are not met

(h) STOT-single exposure;

Based on available data, the classification criteria are not met

(i) STOT-repeated exposure;

Based on available data, the classification criteria are not met

Target Organs

None known.

(j) aspiration hazard;

Based on available data, the classification criteria are not met

Other Adverse Effects

The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed No information available.

11.2. Information on other hazards

Endocrine Disrupting Properties

Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

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SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects

Do not empty into drains. .

Component	Freshwater Fish	Water Flea	Freshwater Algae
Adiponitrile	LC50: = 720 mg/L, 96h static (Lepomis macrochirus) LC50: = 775 mg/L, 96h (Poecilia reticulata) LC50: 1850 - 2020 mg/L, 96h flow-through (Pimephales promelas) LC50: = 820 mg/L, 96h static (Pimephales promelas)	EC50: > 1000 mg/L, 48h (Daphnia magna)	

Component	Microtox	M-Factor
Adiponitrile	EC50 = 393 mg/L 5 min EC50 = 402 mg/L 15 min EC50 = 411 mg/L 30 min	

12.2. Persistence and degradability

Persistence

Readily biodegradable
Persistence is unlikely.

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Adiponitrile	-0.32	No data available

12.4. Mobility in soil

The product is water soluble, and may spread in water systems . Will likely be mobile in the environment due to its water solubility. Highly mobile in soils

12.5. Results of PBT and vPvB assessment

No data available for assessment.

12.6. Endocrine disrupting properties

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects

Persistent Organic Pollutant Ozone Depletion Potential

This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point.

European Waste Catalogue (EWC)

According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

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SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN2205
14.2. UN proper shipping name ADIPONITRILE
14.3. Transport hazard class(es) 6.1
14.4. Packing group III

ADR

14.1. UN number UN2205
14.2. UN proper shipping name ADIPONITRILE
14.3. Transport hazard class(es) 6.1
14.4. Packing group III

IATA

14.1. UN number UN2205
14.2. UN proper shipping name ADIPONITRILE
14.3. Transport hazard class(es) 6.1
14.4. Packing group III

14.5. Environmental hazards No hazards identified
14.6. Special precautions for user No special precautions required
14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

International Inventories

X = listed, Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), China (IECSC), Japan (ENCS), Australia (AICS), Korea (ECL).

Component	EINECS	ELINCS	NLP	TSCA	DSL	NDSL	PICCS	ENCS	IECSC	AICS	KECL
Adiponitrile	203-896-3	-		X	X	-	X	X	X	X	KE-0027 4

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

National Regulations

WGK Classification See table for values

Component	Germany - Water Classification (VwVwS)	Germany - TA-Luft Class
Adiponitrile	WGK1	

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

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15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

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

H301 - Toxic if swallowed

H332 - Harmful if inhaled

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC (volatile organic compound)

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

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Revision Summary Update to CLP Format.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006
COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No
1907/2006**

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

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materials or in any process, unless specified in the text

End of Safety Data Sheet