

# Safety Data Sheet

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifier**

Trade name/designation:	Acetonitrile Gradient -Nmr Tested HPLC
Product No.:	A2096
Synonymes:	Cyanomethane, Ethanenitrile, Ethanoic acid nitrile, Methyl cyanide
CAS No.	75-05-8

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

Relevant identified uses:	General chemical reagent
---------------------------	--------------------------

**1.3 Details of the supplier of the safety data sheet****Supplier****Avantor Performance Materials India Ltd.**

Street	501, 5th floor, Tiffany Building, Hiranandani Business Park,
Postal code/city	Thane, Maharashtra - 400607, India
Telephone	022-41288100

**Emergency phone number**

Telephone	1800105561
-----------	------------

**Preparation Information**

Product Information Compliance

**1.4 E-mail**

SDS@avantorsciences.com

## SECTION 2: Hazard identification

### 2.1 Classification of the substance or mixture

#### Physical hazards

Flammable liquid, category 2

#### health hazards

Acute toxicity, category 4, oral, dermal and inhalation

Eye irritation, category 2

### 2.2 Label elements

#### Hazard pictograms



#### Signal word: Danger

Highly flammable liquid and vapour.

Harmful if swallowed, in contact with skin or if inhaled.

Causes serious eye irritation.

### 2.3 Other hazards none

## SECTION 3: Composition / information on ingredients

### Substances

Substance name	Acetonitrile
Molecular formula	H <sub>3</sub> CCN
Molecular weight	41.05 g/mol
CAS No.	75-05-8

## SECTION 4: First aid measures

### 4.1 General information

IF exposed or if you feel unwell: Call a POISON CENTRE or doctor/physician. If unconscious place in recovery position and seek medical advice. Never give anything by mouth to an unconscious person or a person with cramps. Change contaminated, saturated clothing. Do not leave affected person unattended.

#### After inhalation

Call a POISON CENTRE/doctor. Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

#### In case of skin contact

After contact with skin, wash immediately with plenty of water and soap. Remove contaminated, saturated clothing immediately. In case of skin reactions, consult a physician.

**After eye contact**

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist. Protect uninjured eye. Remove contact lenses, if present and easy to do. Continue rinsing.

**In case of ingestion**

If accidentally swallowed rinse the mouth with plenty of water (only if the person is conscious) and obtain immediate medical attention. Do NOT induce vomiting. Give nothing to eat or drink.

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

no data available

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

no data available

no data available

**SECTION 5: Firefighting measures****5.1 Extinguishing media****Suitable extinguishing media**

Water spray  
ABC-powder  
Carbon dioxide (CO<sub>2</sub>)  
Nitrogen

**Extinguishing media which must not be used for safety reasons**

no restriction

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

In case of fire may be liberated:

Carbon monoxide  
Carbon dioxide (CO<sub>2</sub>)  
Nitrogen oxides (NO<sub>x</sub>)

**5.3 Advice for firefighters**

DO NOT fight fire when fire reaches explosives.  
Special protective equipment for firefighters  
Wear a self-contained breathing apparatus and chemical protective clothing.

**5.4 Additional information**

Do not allow run-off from fire-fighting to enter drains or water courses.  
Do not inhale explosion and combustion gases.  
Use caution when applying carbon dioxide in confined spaces. Carbon dioxide can displace oxygen.  
Use water spray jet to protect personnel and to cool endangered containers.  
In case of fire: Evacuate area.

**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

In case of major fire and large quantities: Remove persons to safety.

**6.2 Environmental precautions**

Discharge into the environment must be avoided.

**6.3 Methods and material for containment and cleaning up**

Spilled product must never be returned to the original container for recycling. Collect in closed and suitable containers for disposal.

**6.4 Additional information**

Clear spills immediately.

**SECTION 7: Handling and storage****Precautions for safe handling**

All work processes must always be designed so that the following is as low as possible:

Inhalation

skin contact

Eye contact

Keep away from sources of ignition - No smoking.

Usual measures for fire prevention.

Take precautionary measures against static discharges.

Protect from moisture.

**Conditions for safe storage, including any incompatibilities**

Recommended storage temperature: Keep bottles tightly closed and away from sources of ignition and heat.

Keep container tightly closed and in a well-ventilated place. Keep/Store away from combustible materials.

**Specific end use(s)**

no data available

**SECTION 8: Exposure controls/personal protection****8.1 Control parameters**

Does not contain substances above concentration limits fixing an occupational exposure limit.

**8.2 Exposure controls****Appropriate engineering controls**

no data available

**Personal protection equipment**

no data available

*Eye/face protection*

no data available

*Skin protection*

Wear suitable gloves. When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. In the case of wanting to use the gloves again, clean them before taking off and air them well. Check leak tightness/impermeability prior to use.

By short-term hand contact

Suitable material:	NBR (Nitrile rubber)
Thickness of the glove material:	0,425 mm
Breakthrough time (maximum wearing time):	14 min

By long-term hand contact

Suitable material:	Butyl caoutchouc (butyl rubber)
Thickness of the glove material:	0,30 mm
Breakthrough time (maximum wearing time):	> 480 min

*Respiratory protection*

no data available

*Additional information*

no data available

*Environmental exposure controls*

no data available

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |                      |                   |
|----------------------|-------------------|
| (a) Appearance       |                   |
| Physical state:      | liquid            |
| Colour:              | colourless        |
| (b) Odour:           | ether-like        |
| (c) Odour threshold: | no data available |

### Safety relevant basic data

- |  |                                     |
|--|-------------------------------------|
| (d) pH:                                      | no data available                   |
| (e) Melting point/freezing point:            | -45.7 °C                            |
| (f) Initial boiling point and boiling range: | 81.6 °C (1013 hPa)                  |
| (g) Flash point:                             | 2 °C (closed cup)                   |
| (h) Evaporation rate:                        | no data available                   |
| (i) Flammability (solid, gas):               | Highly flammable liquid and vapour. |
| (j) Flammability or explosive limits         |                                     |
| Lower explosion limit:                       | 3 % (v/v)                           |
| Upper explosion limit:                       | 17 % (v/v)                          |
| (k) Vapour pressure:                         | 97 hPa (20 °C)                      |
| (l) Vapour density:                          | 1.42 (20 °C)                        |
| (m) Relative density:                        | 0.782 g/cm <sup>3</sup> (20 °C)     |
| (n) Solubility(ies)                          |                                     |
| Water solubility (g/L):                      | soluble (20 °C)                     |
| Soluble (g/L) in Ethanol:                    | no data available                   |
| (o) Partition coefficient: n-octanol/water:  | -0.34 (20 °C; IUCLID)               |
| (p) Auto-ignition temperature:               | 524 °C                              |
| (q) Decomposition temperature:               | no data available                   |
| (r) Viscosity                                |                                     |
| Kinematic viscosity:                         | no data available                   |
| Dynamic viscosity:                           | 0.316 mPa*s (25 °C)                 |
| (s) Explosive properties:                    | not applicable                      |
| (t) Oxidising properties:                    | not applicable                      |

### 9.2 Other information

- |                        |                         |
|------------------------|-------------------------|
| Bulk density:          | no data available       |
| Refraction index:      | 1.34604 (589 nm; 20 °C) |
| Dissociation constant: | no data available       |
| Surface tension:       | no data available       |
| Henry's Law Constant:  | no data available       |

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapours can form explosive mixtures with air.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature).

**10.3 Possibility of hazardous reactions**

Violent reaction with:

Oxidising agent

Reducing agent

Acid

Alkali metals

**10.4 Conditions to avoid**

UV-radiation/sunlight

Heat

This material is combustible and can be ignited by heat, sparks, flames, or other sources of ignition (e.g. static electricity, pilot lights, or mechanical/electrical equipment).

**10.5 Incompatible materials**

Rubber articles

Plastic articles

**10.6 Hazardous decomposition products**

no data available

<b>SECTION 11: Toxicological information</b>
--

**11.1 Information on toxicological effects****Acute effects**

*Acute oral toxicity:*

LD50: < 2730 mg/kg - Rat - (Merck KGaA)

TDLo: > 64 mg/kg - Human

*Acute dermal toxicity:*

LD50: > 988 mg/kg - Rabbit - (IUCAL)

*Acute inhalation toxicity:*

LC50: > 27.3 mg/l (4h) - Rat

**Irritant and corrosive effects**

*Primary irritation to the skin:*

not applicable

*Irritation to eyes:*

Causes serious eye irritation.

*Irritation to respiratory tract:*

not applicable

**Respiratory or skin sensitisation**

In case of skin contact: not sensitising

After inhalation: not sensitising

**STOT-single exposure**

not applicable

**STOT-repeated exposure**

not applicable

**CMR effects (carcinogenicity, mutagenicity and toxicity for reproduction)****Carcinogenicity****Germ cell mutagenicity**

No indications of human germ cell mutagenicity exist.

**Reproductive toxicity**

No indications of human reproductive toxicity exist.

**Aspiration hazard**

not applicable

**Other adverse effects**

no data available

<b>SECTION 12: Ecological information</b>
---

**12.1 Ecotoxicity****Fish toxicity:**

LC50: 1640 mg/l (96 h) - Brooke, L.T., D.J. Call, D.L. Geiger, and C.E. Northcott 1984. Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), Vol. 1. Center for Lake Superior Environmental Stud., Univ. of Wisconsin-Superior, Superior, WI :414

**Daphnia toxicity:**

LC50: 3600 mg/l (48 h) - Tong, Z., Z. Huailan, and J. Hongjun 1996. Chronic Toxicity of Acrylonitrile and Acetonitrile to *Daphnia magna* in 14-d and 21-d Toxicity Tests. Bull. Environ. Contam. Toxicol. 57(4):655-659

**Algae toxicity:**

no data available

**Bacteria toxicity:**

no data available

**12.2 Persistence and degradability**

no data available

**12.3 Bioaccumulative potential**

Partition coefficient: n-octanol/water: -0.34 (20 °C; IUCLID)

**12.4 Mobility in soil:**

no data available

**12.5 Results of PBT/vPvB assessment**

no data available

**12.6 Other adverse effects**

no data available



## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Appropriate disposal / Product

Dispose according to local legislation. Consult the appropriate local waste disposal expert about waste disposal.

#### Appropriate disposal / Package

Dispose according to local legislation. Handle contaminated packages in the same way as the substance itself.

## SECTION 14: Transport information

### Land transport (ADR/RID)

14.1	UN-No.:	1648
14.2	Proper Shipping Name:	ACETONITRILE
14.3	Class(es):	3
	Classification code:	F1
	Hazard label(s):	3
14.4	Packing group:	II
14.5	Environmental hazards:	No
14.6	Special precautions for user:	
	Hazard identification number (Kemler No.):	33
	tunnel restriction code:	D/E
		(Passage forbidden through tunnels of category D when carried in bulk or in tanks. Passage forbidden through tunnels of category E.)

### Sea transport (IMDG)

14.1	UN-No.:	1648
14.2	Proper Shipping Name:	ACETONITRILE
14.3	Class(es):	3
	Classification code:	
	Hazard label(s):	3
14.4	Packing group:	II
14.5	Environmental hazards:	No
	Marine pollutant:	No
14.6	Special precautions for user:	
	Segregation group:	-
	EmS-No.	F-E S-D
14.7	Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	
	not relevant	

**Air transport (ICAO-TI / IATA-DGR)**

14.1	UN-No.:	1648
14.2	Proper Shipping Name:	ACETONITRILE
14.3	Class(es):	3
	Classification code:	
	Hazard label(s):	3
14.4	Packing group:	II
14.5	Special precautions for user:	

## SECTION 15: Regulatory information

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

## SECTION 16: Other information

### Abbreviations and acronyms

ACGIH - American Conference of Governmental Industrial Hygienists  
ADR - European Agreement concerning the International Carriage of Dangerous Goods by Road  
AGS - Committee on Hazardous Substances (Ausschuss für Gefahrstoffe)  
CLP - Regulation on Classification, Labelling and Packaging of Substances and Mixtures  
DFG - German Research Foundation (Deutsche Forschungsgemeinschaft)  
Gestis - Information system on hazardous substances of the German Social Accident Insurance (Gefahrstoffinformationssystem der Deutschen Gesetzlichen Unfallversicherung)  
IATA-DGR - International Air Transport Association-Dangerous Goods Regulations  
ICAO-TI - International Civil Aviation Organization-Technical Instructions  
IMDG - International Maritime Code for Dangerous Goods  
LTV - Long Term Value  
NIOSH - National Institute for Occupational Safety and Health  
OSHA - Occupational Safety & Health Administration  
PBT - Persistent, Bioaccumulative and Toxic  
RID - Regulation concerning the International Carriage of Dangerous Goods by Rail  
STV - Short Term Value  
SVHC - Substances of Very High Concern  
vPvB - very Persistent, very Bioaccumulative

### Additional information

Indication of changes: none

### Disclaimer

The information provided in this Safety Data Sheet (SDS) was prepared based on data believed to be accurate as of the date of this SDS. TO THE GREATEST EXTENT PERMITTED BY LAW, AVANTOR PERFORMANCE MATERIALS ("AVANTOR") EXPRESSLY DISCLAIMS ANY AND ALL REPRESENTATIONS AND WARRANTIES REGARDING THE INFORMATION CONTAINED HEREIN INCLUDING, WITHOUT LIMITATION, AS TO ACCURACY, COMPLETENESS, FITNESS FOR PURPOSE OR USE, MERCHANTABILITY, NON-INFRINGEMENT, PERFORMANCE, SAFETY, SUITABILITY AND STABILITY. This SDS is intended as a guide to the appropriate use, handling, storage and disposal of the product to which it relates by properly trained personnel, and is not intended to be comprehensive. Users of Avantor's products are advised to perform their own tests and to exercise their own judgment to determine the safety, suitability and appropriate use, handling, storage and disposal of each product and product combination for their own purposes and uses. TO THE GREATEST EXTENT PERMITTED BY LAW, AVANTOR DISCLAIMS LIABILITY FOR, AND BY USING AVANTOR'S PRODUCTS THE PURCHASER AGREES THAT UNDER NO CIRCUMSTANCES SHALL AVANTOR BE LIABLE FOR, SPECIAL, INDIRECT, INCIDENTAL, PUNITIVE OR CONSEQUENTIAL DAMAGE OF ANY TYPE OR KIND, INCLUDING WITHOUT LIMITATION, FOR LOSS OF PROFITS, REPUTATIONAL DAMAGE, PRODUCT RECALL OR BUSINESS INTERRUPTION.