

## Material Safety Data Sheet

Date Printed: 16/DEC/2004

Date Updated: 14/MAR/2004

Version 1.2

According to 91/155/EEC

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1 - Product and Company Information

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Product Name	CHLOROACETONITRILE
Product Number	22830
Company	Sigma-Aldrich Pte Ltd #08-01 Citilink Warehouse Singapore 118529 Singapore
Technical Phone #	65 271 1089
Fax	65 271 1571

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2 - Composition/Information on Ingredients

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Product Name	CAS #	EC no	Annex I Index Number
CHLOROACETONITRILE	107-14-2	203-467-0	608-008-00-1
Formula	C2H2ClN		
Molecular Weight	75.5 AMU		
Synonyms	Chloroacetonitrile * alpha-Chloroacetonitrile * 2-Chloroacetonitrile * Chloromethyl cyanide * Monochloroacetonitrile * Monochloromethyl cyanide * USAF KF-5		

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3 - Hazards Identification

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## SPECIAL INDICATION OF HAZARDS TO HUMANS AND THE ENVIRONMENT

Toxic by inhalation, in contact with skin and if swallowed. Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

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4 - First Aid Measures

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## AFTER INHALATION

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

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5 - Fire Fighting Measures

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## EXTINGUISHING MEDIA

Suitable: Carbon dioxide, dry chemical powder, or appropriate foam.

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## SPECIAL RISKS

Specific Hazard(s): Emits toxic fumes under fire conditions.

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## SPECIAL PROTECTIVE EQUIPMENT FOR FIREFIGHTERS

Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.

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## 6 - Accidental Release Measures

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PERSONAL PRECAUTION PROCEDURES TO BE FOLLOWED IN CASE OF LEAK OR SPILL  
Evacuate area.

PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP

Absorb on sand or vermiculite and place in closed containers for disposal.

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7 - Handling and Storage

HANDLING

Directions for Safe Handling: Do not breathe vapor. Do not get in eyes, on skin, on clothing. Avoid prolonged or repeated exposure.

STORAGE

Conditions of Storage: Keep tightly closed. Keep away from heat and open flame. Store in a cool dry place.

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8 - Exposure Controls / Personal Protection

ENGINEERING CONTROLS

Use only in a chemical fume hood. Safety shower and eye bath.

GENERAL HYGIENE MEASURES

Wash thoroughly after handling. Wash contaminated clothing before reuse.

PERSONAL PROTECTIVE EQUIPMENT

Special Protective Measures: Wear appropriate government approved respirator, chemical-resistant gloves, safety goggles, other protective clothing.

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9 - Physical and Chemical Properties

Appearance	Color: Yellow Form: Clear liquid	
Property	Value	At Temperature or Pressure
pH	N/A	
BP/BP Range	123 - 125 °C	
MP/MP Range	N/A	
Flash Point	54 °C	Method: closed cup
Flammability	N/A	
Autoignition Temp	N/A	
Oxidizing Properties	N/A	
Explosive Properties	N/A	
Explosion Limits	N/A	
Vapor Pressure	15 mmHg	30 °C
SG/Density	1.196 g/cm <sup>3</sup>	
Partition Coefficient	Log Kow: 0.45	
Viscosity	N/A	
Vapor Density	3 g/l	
Saturated Vapor Conc.	N/A	
Evaporation Rate	N/A	
Bulk Density	N/A	
Decomposition Temp.	N/A	

Solvent Content	N/A
Water Content	N/A
Surface Tension	N/A
Conductivity	N/A
Miscellaneous Data	N/A
Solubility	Solubility in Water: Insoluble. Other Solvents: HYDROCARBONS, ALCOHOLS

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## 10 - Stability and Reactivity

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### STABILITY

Materials to Avoid: Strong acids, Strong bases, Strong oxidizing agents, Strong reducing agents.

### HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Thermal decomposition may produce carbon monoxide, carbon dioxide, and nitrogen oxides.

### HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

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## 11 - Toxicological Information

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RTECS NUMBER: AL8225000

### ACUTE TOXICITY

LD50  
Oral  
Rat  
220 mg/kg

LD50  
Oral  
Mouse  
139 mg/kg

LD50  
Intraperitoneal  
Mouse  
100 MG/KG

LD50  
Skin  
Rabbit  
71 UL/KG

### IRRITATION DATA

Skin  
Rabbit  
14 mg  
24H  
Remarks: Open irritation test

Skin  
Rabbit  
500 mg  
24H  
Remarks: Mild irritation effect

Eyes

Rabbit  
20 mg  
24H  
Remarks: Moderate irritation effect

#### SIGNS AND SYMPTOMS OF EXPOSURE

Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea, and vomiting. May cause cyanosis (blue-gray coloring of skin and lips caused by lack of oxygen). To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

#### ROUTE OF EXPOSURE

Skin Contact: May cause skin irritation.  
Skin Absorption: Toxic if absorbed through skin.  
Eye Contact: May cause eye irritation.  
Inhalation: Toxic if inhaled. Material may be irritating to mucous membranes and upper respiratory tract.  
Ingestion: Toxic if swallowed.

#### CHRONIC EXPOSURE - CARCINOGEN

Mouse  
Route of Application: Skin  
Exposure Time: 2W  
Result: Tumorigenic: Carcinogenic by RTECS criteria. Skin and Appendages: Other: Tumors.

#### IARC CARCINOGEN LIST

Rating: Group 3

#### CHRONIC EXPOSURE - MUTAGEN

Human  
15 UMOL/L  
Cell Type: lymphocyte  
DNA damage

Rat  
115 MG/KG  
Oral  
Unscheduled DNA synthesis

Hamster  
79100 NMOL/L  
Cell Type: ovary  
Sister chromatid exchange

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#### 12 - Ecological Information

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#### ECOTOXICOLOGICAL EFFECTS

Test Type: LC50 Fish  
Species: Pimephales promelas (Fathead minnow)  
Time: 96 h  
Value: 1.15 - 1.580 mg/l

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#### 13 - Disposal Considerations

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#### SUBSTANCE DISPOSAL

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

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## 14 - Transport Information

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### RID/ADR

UN#: 2668  
Class: 6.1  
PG: II  
Proper Shipping Name: Chloroacetonitrile

### IMDG

UN#: 2668  
Class: 6.1  
PG: II  
Subrisk: 3  
Proper Shipping Name: Chloroacetonitrile  
Marine Pollutant: No  
Severe Marine Pollutant: No

### IATA

UN#: 2668  
Class: 6.1  
PG: II  
Subrisk: 3  
Proper Shipping Name: Chloroacetonitrile  
Inhalation Packing Group I: Yes

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## 15 - Regulatory Information

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### CLASSIFICATION AND LABELING ACCORDING TO EU DIRECTIVES

ANNEX I INDEX NUMBER: 608-008-00-1

INDICATION OF DANGER: T N

Toxic. Dangerous for the environment.

R-PHRASES: 23/24/25 51/53

Toxic by inhalation, in contact with skin and if swallowed.

Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

S-PHRASES: 45 61

In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Avoid release to the environment. Refer to special instructions/safety data sheets.

### SWITZERLAND

SWISS POISON CLASS: 2

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## 16 - Other Information

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### WARRANTY

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. Copyright 2004 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.

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