Chemical Safety Data Sheet MSDS / SDS

2-hydroxy-2-methylpropionitrile SDS

Revision Date:2024-04-25 Revision Number:1

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

Product identifier

Product name: 2-hydroxy-2-methylpropionitrile

CAS: 75-86-5

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

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.

Uses advised against: none

Company Identification

Company: Chemicalbook.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

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SECTION 2: Hazards identification

Classification of the substance or mixture

Acute toxicity - Category 2, Oral
Acute toxicity - Category 1, Dermal

Acute toxicity - Category 2, Inhalation
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H300 Fatal if swallowed
H310 Fatal in contact with skin
H330 Fatal if inhaled
H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P262 Do not get in eyes, on skin, or on clothing.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P284 [In case of inadequate ventilation] wear respiratory protection.
P273 Avoid release to the environment.

Response

P301+P316 IF SWALLOWED: Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P316 Get emergency medical help immediately.
P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P320 Specific treatment is urgent (see ... on this label).
P391 Collect spillage.

Storage

P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	2-hydroxy-2-methylpropionitrile
Common names and synonyms:	2-hydroxy-2-methylpropionitrile
CAS number:	75-86-5
EC number:	200-909-4
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Half-upright position. Artificial respiration may be needed. Refer for medical attention.

Following skin contact

Rinse and then wash skin with water and soap. Refer for medical attention .

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Refer for medical attention .

Most important symptoms/effects, acute and delayed

This material is considered very hazardous and should only be handled under conditions that prevent any inhalation of vapor or skin contact. May be slightly irritating to skin and mucous membranes. (EPA, 1998)

Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Remove patient from contact with the material. Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Cyanide and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water. Use "alcohol" foam, dry chemical or carbon dioxide. Keep run-off water out of sewers and water sources.

Specific hazards arising from the chemical

Too dangerous to health to expose fire fighters; a few whiffs of vapor could cause death; vapor or liquid could be fatal on penetrating normal protective clothing. Vapor forms explosive mixture with air. Decomposes when heated to 248F or at lower temperature under alkaline conditions, emitting highly toxic hydrogen cyanide. May react violently with water. Contact with sulfuric acid may cause it to explode. (EPA, 1998)

Special protective actions for fire-fighters

Use powder, AFFF, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water. NO direct contact with water. Combat fire from a sheltered position.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: complete protective clothing including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: complete protective clothing including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. Carefully collect remainder. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Releases may require isolation or evacuation. Use water spray to cool and disperse vapors, protect personnel, and dilute spills to form nonflammable mixtures. Control runoff and isolate discharged material for proper disposal.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Above 74°C use a closed system and ventilation. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Provision to contain effluent from fire extinguishing. Separated from strong bases, acids, water and food and feedstuffs. Well closed. Keep in a well-ventilated room.Separate from acids, alkalies, oxidizing materials, and reducing agents. Store in a cool, dry, well-ventilated location.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 5 mg/m3 (ceiling value); (skin)

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear face shield or eye protection in combination with breathing protection.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use closed system or ventilation.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Liquid.
Colour:	Colourless to yellowish, clear.
Odour:	Distinct strong cyanide odor
Melting point/freezing point:	-19 °C.
Boiling point or initial boiling point and boiling range:	82 °C. Atm. press.:31 hPa.
Flammability:	Class IIIA Combustible Liquid: Fl.P. at or above 140°F and below 200°F.

Lower and upper explosion limit/flammability limit:	Lower flammable limit: 2.2% by volume; Upper flammable limit:12.0% by volume
Flash point:	75 °C. Atm. press.:1 013 hPa.
Auto-ignition temperature:	540 °C. Atm. press.:1 013 hPa. Remarks:Atmospheric pressure: unspecified, but we assume it to be 1013 hPa.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	greater than or equal to 100 mg/mL at 68° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Pow = -1. Remarks:Calculated according to Rekker (hydrophobic?fragmental?constant? method).
Vapour pressure:	0.3 hPa. Temperature:20 °C.
Density and/or relative density:	0.93 g/cm3. Temperature:20 °C.
Relative vapour density:	2.93 (EPA, 1998) (Relative to Air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes rapidly on heating and on contact with bases and water. This produces highly toxic and flammable hydrogen cyanide (see ICSC 0492) and acetone (see ICSC 0087). Reacts violently with acids and oxidants. This generates fire and explosion hazard.

Chemical stability

no data available

Possibility of hazardous reactions

Combustible liquidThe vapour is heavier than air.ACETONE CYANOHYDRIN readily decomposes to acetone and poisonous hydrogen cyanide gas on contact with water, acids (sulfuric acid) or when exposed to heat. Should be kept cool and slightly acidic (pH 4-5) [Sax, 2nd ed., 1965, p. 388]. Slowly dissociates to acetone, a flammable liquid, and hydrogen cyanide, a flammable poisonous gas, under normal storage and transportation conditions. Rate of dissociation increased by contact with alkalis and/or heat.

Conditions to avoid

no data available

Incompatible materials

Sulfuric acid, caustics [Note: Slowly decomposes to acetone & HCN at room temperatures; rate is accelerated by an increase in pH, water content, or temperature].

Hazardous decomposition products

When heated to decomposition it emits toxic fumes of /hydrogen cyanide/.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male) - 0.017 mL/kg bw. Remarks:Original value.

Inhalation: LCLo - rat - 62.5 ppm.

Dermal: LD50 - rabbit (male/female) - 16 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes, skin and respiratory tract. The substance may cause effects on the cardiovascular system and central nervous system. This may result in asphyxia, cardiac disorders, convulsions, cyanosis and respiratory failure. Exposure could cause death. Medical observation is indicated. See Notes.

STOT-repeated exposure

The substance may have effects on the central nervous system and thyroid. This may result in impaired functions.

Aspiration hazard

A harmful contamination of the air can be reached rather quickly on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Oncorhynchus mykiss (previous name: Salmo gairdneri) - 0.22 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 0.13 mg/L - 48 h.

Toxicity to algae: LOEC - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - 0.16 mg/L - 96 h.

Toxicity to microorganisms: EC50 - Vibrio fisheri - 21 mg/L - 15 min.

Persistence and degradability

AEROBIC: Acetone cyanohydrin was only partially biodegradable in aqueous activated sludge screening tests by the standard bottle dilution method(1). Acetone cyanohydrin, present at 100 mg/L, reached 53-64% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test which classified the compound as readily biodegradable(2). Acetone cyanohydrin dissociates in water (an equilibrium reaction), with half-life of 9 minutes at neutral pH, to form acetone and hydrogen cyanide(3); using the same Japanese MITI test, acetone has theoretical BOD of 98%(2) which might suggest the presence of hydrogen cyanide decreases the biodegradation rate with respect to acetone cyanohydrin in this test(SRC).

Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for acetone cyanohydrin(SRC), using an estimated log Kow of -0.03(1) and a regression-derived equation(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC). In addition, acetone cyanohydrin dissociates in water, 4.47 1/hr (half-life 9 minutes)(3), so bioconcentration in aquatic organisms will not be an important process(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of acetone cyanohydrin can be estimated to be 1(SRC). According to a classification scheme(2), this estimated Koc value suggests that acetone cyanohydrin is expected to have very high mobility in soil. However, if released to soil, based on a hydrolysis rate of 4.47 1/hr (half-life 9 minutes) at pH 7.02 at 26 deg C(3), acetone cyanohydrin will dissociate rapidly with water forming acetone and hydrogen cyanide(3) and make it unlikely that the parent acetone cyanohydrin will be the mobile compound(SRC).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN1541 (For reference only, please check.)
IMDG: UN1541 (For reference only, please check.)
IATA: UN1541 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ACETONE CYANOHYDRIN, STABILIZED (For reference only, please check.)
IMDG: ACETONE CYANOHYDRIN, STABILIZED (For reference only, please check.)
IATA: ACETONE CYANOHYDRIN, STABILIZED (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)
IMDG: 6.1 (For reference only, please check.)
IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)
IMDG: I (For reference only, please check.)
IATA: I (For reference only, please check.)

Environmental hazards

ADR/RID: Yes
IMDG: Yes
IATA: Yes

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

ECHA - European Chemicals Agency, website: https://echa.europa.eu/

Other Information

The occupational exposure limit value should not be exceeded during any part of the working exposure.Specific treatment is necessary in case of poisoning with this substance; the appropriate means with instructions must be available.Hazard and toxicity of this substance is due to its major metabolite - hydrogen cyanide (see ICSC 0492).

Disclaimer: 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. We as supplier shall not be held liable for any