

Chemical Safety Data Sheet MSDS / SDS

Dichloroacetonitrile

Revision Date:2024-12-21 Revision Number:1

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

Product identifier

Product name : Dichloroacetonitrile
CBnumber : CB7853456
CAS : 3018-12-0
EINECS Number : 221-159-4
Synonyms : dichloroacetonitrile

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
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification

Classification of the substance or mixture

Flammable liquids, Category 3
Acute toxicity - Category 4, Oral
Skin corrosion, Sub-category 1B

Label elements

Pictogram(s)

□□□□

Signal word : Danger

Hazard statement(s)

H226 Flammable liquid and vapour
H302 Harmful if swallowed
H314 Causes severe skin burns and eye damage
H318 Causes serious eye damage
H341 Suspected of causing genetic defects
H361 Suspected of damaging fertility or the unborn child

Precautionary statement(s)

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

P233 Keep container tightly closed.

P240 Ground/bond container and receiving equipment.

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P264 Wash hands thoroughly after handling.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P310 Immediately call a POISON CENTER or doctor/physician.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P405 Store locked up.

P403+P235 Store in a well-ventilated place. Keep cool.

P501 Dispose of contents/container to.....

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P233 Keep container tightly closed.

P240 Ground and bond container and receiving equipment.

P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.

P242 Use non-sparking tools.

P243 Take action to prevent static discharges.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].

P370+P378 In case of fire: Use ... to extinguish.

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P363 Wash contaminated clothing before reuse.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P316 Get emergency medical help immediately.

P321 Specific treatment (see ... on this label).

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.

P405 Store locked up.

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

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: Dichloroacetonitrile
Synonyms	: dichloroacetonitrile
CAS	: 3018-12-0
EC number	: 221-159-4
MF	: C ₂ HCl ₂ N
MW	: 109.94

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately.

Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms and effects, both acute and delayed

ACUTE/CHRONIC HAZARDS: When heated to decomposition this chemical emits toxic fumes of chlorine, cyanides and nitrogen oxides. (NTP, 1992)

Indication of any immediate medical attention and special treatment needed

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

Extinguishing media

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

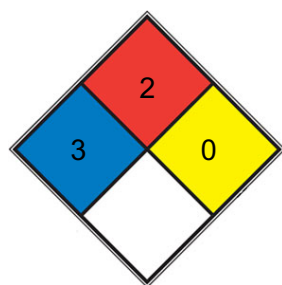
Specific Hazards Arising from the Chemical

This chemical is probably combustible. (NTP, 1992)

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

NFPA 704



<input checked="" type="checkbox"/> HEALTH	3	Short exposure could cause serious temporary or moderate residual injury (e.g. liquid hydrogen , sulfuric acid , calcium hypochlorite , hexafluorosilicic acid)
<input checked="" type="checkbox"/> FIRE	2	Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, sulfur)
<input checked="" type="checkbox"/> REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N2)
<input type="checkbox"/> SPEC.		
<input type="checkbox"/> HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Cover with dry-lime, sand, or soda ash. Place in covered containers using non-sparking tools and transport outdoors. Ventilate area and wash spill site after material pickup is complete.

SECTION 7: Handling and storage

Precautions for safe handling

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

Keep tightly closed. Keep away from heat, sparks, and open flame.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure 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

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	neat
Colour	Liquid
Odour	no data available
Melting point/freezing point	82°C(lit.)
Boiling point or initial boiling point and boiling range	112°C(lit.)
Flammability	no data available

Lower and upper explosion limit/flammability limit	no data available
Flash point	35°C(lit.)
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	10 to 50 mg/mL at 70.7° F (NTP, 1992)
Partition coefficient n-octanol/water	log Kow = 0.29 (est)
Vapour pressure	2.82 mm Hg at 25 deg C (est)
Density and/or relative density	1.37
Relative vapour density	1.37
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

Burns slowly, emitting a thick black smoke, but will not flash (NTP, 1992). Water soluble.

Chemical stability

no data available

Possibility of hazardous reactions

DICHLOROACETONITRILE is a halogenated nitrile. Nitriles may polymerize in the presence of metals and some metal compounds. They are incompatible with acids; mixing nitriles with strong oxidizing acids can lead to extremely violent reactions. Nitriles are generally incompatible with other oxidizing agents such as peroxides and epoxides. The combination of bases and nitriles can produce hydrogen cyanide. Nitriles are hydrolyzed in both aqueous acid and base to give carboxylic acids (or salts of carboxylic acids). These reactions generate heat. Peroxides convert nitriles to amides. Nitriles can react vigorously with reducing agents.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits toxic fumes of /Hydrogen Chloride/, /Cyanide/, and /Nitrogen oxides/.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Mouse (male) oral 270 mg/kg[Hayes JR et al; Environ Health Perspect 69: 183-202 (1986)] Full text: PMC1474335

- Inhalation: no data available
- Dermal: no data available

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

Evaluation: No epidemiological data relevant to the carcinogenicity of dichloroacetonitrile were available. There is inadequate evidence in experimental animals for the carcinogenicity of dichloroacetonitrile. Overall evaluation: Dichloroacetonitrile is not classifiable as to its carcinogenicity to humans (Group 3).

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

Dichloroacetonitrile is a by product of water chlorination and hydrolyzes quickly, therefore biodegradation is not expected to be an important fate in the environment. (SRC)

Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for dichloroacetonitrile(SRC), using an estimated log Kow of 0.29(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of dichloroacetonitrile can be estimated to be 13(SRC). According to a classification scheme(2), this estimated Koc value suggests that dichloroacetonitrile is expected to have very high mobility in soil.

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: UN2920 (For reference only, please check.)

IMDG: UN2920 (For reference only, please check.)

IATA: UN2920 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: CORROSIVE LIQUID, FLAMMABLE, N.O.S. (For reference only, please check.)

IMDG: CORROSIVE LIQUID, FLAMMABLE, N.O.S. (For reference only, please check.)

IATA: CORROSIVE LIQUID, FLAMMABLE, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 8 (For reference only, please check.)

IMDG: 8 (For reference only, please check.)

IATA: 8 (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: No

IMDG: No

IATA: No

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

Not Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

PICCS

Not Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Not Listed.

Korea Existing Chemicals List (KECL)

Not 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?pagelD=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/>

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