Chemical Safety Data Sheet MSDS / SDS

1,3-Acetonedicarboxylic acid

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

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

Product identifier

Product name	: 1,3-Acetonedicarboxylic acid	
CBnumber	: CB1710881	
CAS	: 542-05-2	
EINECS Number	: 208-797-9	
Synonyms	: 3-oxopentanedioic acid, 1, 3-ACETONEDICARBOXYLIC ACID	
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

Skin irritation, Category 2 Eye irritation, Category 2

Label elements

Pictogram(s)

Signal word

Warning

Hazard statement(s)

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

Precautionary statement(s)

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P264 Wash hands thoroughly after handling.

P264 Wash skin thouroughly after handling.

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P280 Wear protective gloves/protective clothing/eye protection/face protection. P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing. P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing. P405 Store locked up. Prevention P264 Wash ... thoroughly after handling. P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/... Response P302+P352 IF ON SKIN: Wash with plenty of water/... P321 Specific treatment (see ... on this label). P332+P317 If skin irritation occurs: Get medical help. P362+P364 Take off contaminated clothing and wash it before reuse. 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 none Disposal none Other hazards no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: 1,3-Acetonedicarboxylic acid
Synonyms	: 3-oxopentanedioic acid,1,3-ACETONEDICARBOXYLIC ACID
CAS	: 542-05-2
EC number	: 208-797-9
MF	: C5H6O5
MW	: 146.1

SECTION 4: First aid measures

Description of first aid measures

lf 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

no data available

Indication of any immediate medical attention and special treatment needed

no data available

SECTION 5: Firefighting measures

Extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam.

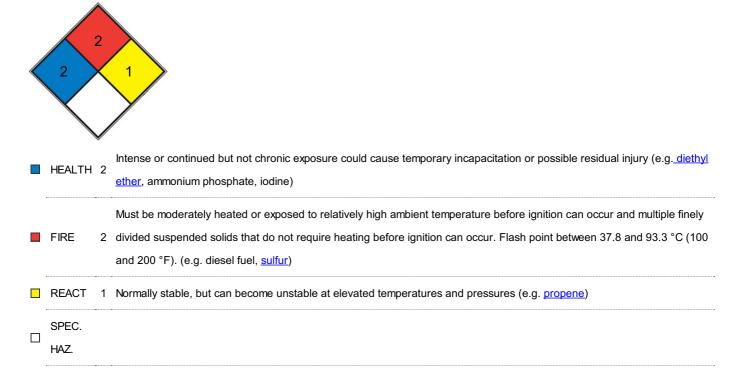
Specific Hazards Arising from the Chemical

no data available

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

NFPA 704



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

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use sparkproof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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 riskelimination 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.

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	Crystalline Powder
Colour	White
Odour	no data available
Melting point/freezing point	138 °C. Atm. press.:990 hPa.
Boiling point or initial boiling point and	300 °C. Atm. press.:990 hPa.
boiling range	
Flammability	no data available
Lower and upper explosion	no data available
limit/flammability limit	
Flash point	200 °C. Atm. press.:990 hPa.
Auto-ignition temperature	Remarks:Does not catch fire at room temperature and pressure. Thereby, it can be inferred that the
	chemical is not autoflammable.
Decomposition temperature	no data available
рН	2.1. Remarks:Acidic.
Kinematic viscosity	no data available
Solubility	DMSO (Slightly, Heated), Methanol (Slightly)
Partition coefficient n-octanol/water	Pow = 0.316. Temperature:30 °C. Remarks:Log Pow = -0.500.
Vapour pressure	0 mm Hg. Remarks:(Modified Grain Method).
Density and/or relative density	0.6 g/cm3. Temperature:30 °C.
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 mouse 6 000 mg/kg bw. Remarks: Tumorigenic active as anti-cancer agent.
- Inhalation: LC0 rat 5.7 mg/L air.
- Dermal: LD50 rabbit > 10 000 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

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Pimephales promelas - 1 000 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: LC50 - Daphnia magna - 1 000 mg/L - 48 h.

Toxicity to algae: EC50 - green algae - 153 000 mg/L - 96 h.

Toxicity to microorganisms: IGC50 - Tetrahymena pyriformis - 2 283.759 mg/L - 46 h.

Persistence and degradability

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

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: Not dangerous goods. (For reference only, please check.) IMDG: Not dangerous goods. (For reference only, please check.) IATA: Not dangerous goods. (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.) IMDG: Not dangerous goods. (For reference only, please check.) IATA: Not dangerous goods. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.) IMDG: Not dangerous goods. (For reference only, please check.) IATA: Not dangerous goods. (For reference only, please check.)

Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.) IMDG: Not dangerous goods. (For reference only, please check.) IATA: Not dangerous goods. (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 Listed. China Catalog of Hazardous chemicals 2015 Not Listed. New Zealand Inventory of Chemicals (NZIoC) Listed. PICCS Listed. **Vietnam National Chemical Inventory** Listed. IECSC Not Listed. Korea Existing Chemicals List (KECL) Listed.

SECTION 16: Other information

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

ChemlDplus, 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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