

SAFETY DATA SHEET

according to the OSHA
Hazard Communication Standard

Version 6.18
Revision Date 07/15/2026
Print Date 07/16/2026

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : *cis*-Aconitic acid

Product Number : A3412
Brand : Aldrich
CAS-No. : 585-84-2

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

Identified uses : Laboratory chemicals, Synthesis of substances

Restrictions on use : After February 3, 2025, this chemical substance (as defined in TSCA section 3(2))/product cannot be distributed in commerce to retailers. After January 28, 2026, this chemical substance (as defined in TSCA section 3(2))/product is and can only be distributed in commerce or processed with a concentration of methylene chloride equal to or greater than 0.1% by weight for the following purposes: (1) Processing as a reactant; (2) Processing for incorporation into a formulation, mixture, or reaction product; (3) Processing for repackaging; (4) Processing for recycling; (5) Industrial or commercial use as a laboratory chemical; (6) Industrial or commercial use as a bonding agent for solvent welding; (7) Industrial and commercial use as a paint and coating remover from safety critical, corrosion-sensitive components of aircraft and spacecraft; (8) Industrial and commercial use as a processing aid; (9) Industrial and commercial use for plastic and rubber products manufacturing; (10) Industrial and commercial use as a solvent that becomes part of a formulation or mixture, where that formulation or mixture will be used inside a manufacturing process, and the solvent (methylene chloride) will be reclaimed; (11) Industrial and commercial use in the refinishing for wooden furniture, decorative pieces, and architectural fixtures of artistic, cultural or historic value until May 8, 2029; (12) Industrial and commercial use in adhesives and sealants in aircraft, space vehicle, and turbine applications for structural and safety critical non-structural applications until May 8, 2029; (13) Disposal; and (14) Export.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Skin irritation : Category 2

Eye irritation : Category 2A

Carcinogenicity : Category 1B

Specific target organ toxicity - single exposure : Category 3 (Respiratory system)

Other hazards

May form explosive peroxides.

GHS label elements

Hazard pictograms :



Signal word : Danger

Hazard statements : H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.
H350 May cause cancer.

Precautionary statements : **Prevention:**
P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P261 Avoid breathing dust.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.

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

Response:

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.

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

P308 + P313 IF exposed or concerned: Get medical advice/ attention.

P332 + P313 If skin irritation occurs: Get medical advice/ attention.

P337 + P313 If eye irritation persists: Get medical advice/ attention.

P362 Take off contaminated clothing and wash before reuse.

Storage:

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

P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 585-84-2

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
cis-Aconitic acid	585-84-2*	>= 80 - <= 100	TSC
Dichloromethane	75-09-2*	>= 1 - <= 5	TSC
1,4-Dioxane	123-91-1*	>= 1 - <= 5	TSC

* Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice	: Show this safety data sheet to the doctor in attendance.
If inhaled	: After inhalation: fresh air. Call in physician.
In case of skin contact	: In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.
In case of eye contact	: After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.
If swallowed	: After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.
Most important symptoms and effects, both acute and delayed	: The most important known symptoms and effects are described in the labelling (see section 2 GHS label elements) and/or in section 11
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO ₂) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible. Mixture with combustible ingredients. Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion	: Carbon oxides

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products

Hydrogen chloride gas

- | | | |
|--|---|--|
| Specific extinguishing methods | : | No data available |
| Further information | : | Suppress (knock down) gases/vapours/mists with a water spray jet.
Prevent fire extinguishing water from contaminating surface water or the ground water system. |
| Special protective equipment for fire-fighters | : | Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing. |

SECTION 6. ACCIDENTAL RELEASE MEASURES

- | | | |
|---|---|---|
| Personal precautions, protective equipment and emergency procedures | : | Advice for non-emergency personnel:
Avoid generation and inhalation of dusts in all circumstances.
Avoid substance contact.
Ensure adequate ventilation.
Evacuate the danger area, observe emergency procedures, consult an expert.
Advice for emergency responders:
Wear appropriate personal protective equipment, as indicated in Section 8. |
| Environmental precautions | : | Do not let product enter drains. |
| Methods and materials for containment and cleaning up | : | Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10).
Take up carefully. Dispose of properly. Clean up affected area.
Avoid generation of dusts. |

SECTION 7. HANDLING AND STORAGE

For precautions see section 2 GHS label elements

- | | | |
|-------------------------|---|---|
| Advice on safe handling | : | Work under hood. Do not inhale substance/mixture. |
|-------------------------|---|---|

Further information on storage conditions : Tightly closed.
Dry.
Keep in a well-ventilated place.
Keep locked up or in an area accessible only to qualified or authorised persons.

Storage class : 6.1C, Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

Recommended storage temperature : -4 °F / -20 °C

/

Further information on storage stability : Test for peroxide formation periodically and before distillation.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
Dichloromethane	75-09-2	TWA	50 ppm	ACGIH
		PEL	25 ppm	OSHA CARC
		STEL	125 ppm	OSHA CARC
		ECEL-TWA	2 ppm 8 mg/m ³	TSCA ECEL
		EPA STEL	16 ppm 57 mg/m ³	TSCA ECEL
1,4-Dioxane	123-91-1	TWA	20 ppm	ACGIH
		TWA	25 ppm 90 mg/m ³	OSHA P0
		TWA	100 ppm 360 mg/m ³	OSHA Z-1
		C	1 ppm 3.6 mg/m ³	NIOSH REL

Biological occupational exposure limits

Components	CAS-No.	Control parameters	Biological specimen	Sampling time	Permissible concentration	Basis
Dichloromethane	75-09-2	Dichloromethane	Urine	End of shift (As	0.3 mg/l	ACGIH BEI

				soon as possible after exposure ceases)		
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Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type P3

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Full contact
Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Splash contact
Manufacturer : KCL 741 Dermatril® L

Remarks : Handle with impervious gloves.
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-

- Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Safety glasses
- Skin and body protection : protective clothing
- Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

- Appearance : solid
- Colour : No data available
- Odour : No data available
- Odour Threshold : No data available
pH : No data available
- Melting point/ range : 252 °F / 122 °C
Method: lit.
- Boiling point/boiling range : No data available
- Flash point : Not applicable
- Evaporation rate : No data available
- Flammability (solid, gas) : No data available
- Flammability (liquids) : No data available
- Burning rate : No data available
- Upper explosion limit /
Upper flammability limit : No data available
- Lower explosion limit /
Lower flammability limit : No data available
- Vapour pressure : No data available
- Relative vapour density : No data available
- Relative density : No data available

Density	: No data available
Water solubility	: No data available
Partition coefficient: n-octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Molecular weight	: 174.11 g/mol
Particle characteristics	
Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Formation of peroxides possible.
	The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: Violent reactions possible with: Strong oxidizing agents
Conditions to avoid	: Moisture.
Incompatible materials	: No data available
Hazardous decomposition products	: Peroxides
	: In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - > 5,000 mg/kg
(Calculation method)
Inhalation: No data available
Acute toxicity estimate Dermal - > 5,000 mg/kg
(Calculation method)

Skin corrosion/irritation

Remarks: Causes skin irritation.

Serious eye damage/eye irritation

Remarks: Causes serious eye irritation.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: 2A - Group 2A: Probably carcinogenic to humans (Dichloromethane)
IARC: 2B - Group 2B: Possibly carcinogenic to humans (1,4-Dioxane)
NTP: RAHC - Reasonably anticipated to be a human carcinogen (Dichloromethane)
NTP: RAHC - Reasonably anticipated to be a human carcinogen (1,4-Dioxane)
OSHA: OSHA specifically regulated carcinogen (Dichloromethane)

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

Dichloromethane:

Toxicity to fish	: LC50 (Pimephales promelas (fathead minnow)): 193.00 mg/l End point: mortality Exposure time: 96 h Test Type: flow-through test Analytical monitoring: yes Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	: LC50 (Daphnia magna (Water flea)): 27 mg/l End point: mortality Exposure time: 48 h Test Type: static test Method: US-EPA
Toxicity to fish (Chronic toxicity)	: LC50 (Pimephales promelas (fathead minnow)): 471 mg/l End point: mortality Exposure time: 8 d Test Type: flow-through test Analytical monitoring: yes Remarks: (ECHA)
Toxicity to microorganisms	: EC50 (activated sludge): 2,590 mg/l Exposure time: 40 min Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 209

1,4-Dioxane:

Toxicity to daphnia and other aquatic invertebrates	: EC50 (Daphnia magna (Water flea)): > 1,000 mg/l End point: Immobilization Exposure time: 48 h Test Type: semi-static test Analytical monitoring: yes Method: OECD Test Guideline 202 GLP: yes
Toxicity to algae/aquatic plants	: ErC50 (Pseudokirchneriella subcapitata (green algae)): > 1,000 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes

Toxicity to fish (Chronic toxicity) : NOEC (Pimephales promelas (fathead minnow)): > 103 mg/l
 End point: mortality
 Exposure time: 32 d
 Test Type: flow-through test
 Analytical monitoring: yes
 GLP: yes
 Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : NOEC (Daphnia magna (Water flea)): 1,000 mg/l
 End point: reproduction rate
 Exposure time: 21 d
 Method: OECD Test Guideline 211

Persistence and degradability

Components:

Dichloromethane:

Biodegradability : aerobic
 Inoculum: activated sludge, non-adapted
 Concentration: 5 mg/l
 Result: Readily biodegradable.
 Biodegradation: 68 %
 Exposure time: 28 d
 Method: OECD Test Guideline 301D
 GLP: yes

1,4-Dioxane:

Biodegradability : aerobic
 Inoculum: activated sludge
 Concentration: 100 mg/l
 Result: Not readily biodegradable.
 Biodegradation: < 10 %
 Exposure time: 29 d
 Method: OECD Test Guideline 301F

Bioaccumulative potential

Components:

Dichloromethane:

Bioaccumulation : Species: Cyprinus carpio (Carp)
 Bioconcentration factor (BCF): 2 - 5.4
 Exposure time: 6 Weeks
 Concentration: 250 µg/l
 Method: OECD Test Guideline 305
 GLP: yes

Species: Cyprinus carpio (Carp)
 Bioconcentration factor (BCF): 6 - 40
 Exposure time: 6 Weeks

Concentration: 25 µg/l
Method: OECD Test Guideline 305
GLP: yes

Partition coefficient: n-octanol/water : log Pow: 1.25 (68 °F / 20 °C)
pH: 7
Method: (experimental)
Remarks: Bioaccumulation is not expected.

1,4-Dioxane:

Bioaccumulation : Species: Cyprinus carpio (Carp)
Bioconcentration factor (BCF): 0.3 - 0.7
Temperature: 77 °F / 25 °C
Concentration: 10 mg/l
Method: OECD Test Guideline 305C

Partition coefficient: n-octanol/water : log Pow: -0.42
Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Components:

Dichloromethane:

Results of PBT and vPvB assessment : Not persistent, bioaccumulative, and toxic (PBT). Not very persistent and very bioaccumulative (vPvB).
: Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

1,4-Dioxane:

Additional ecological information : Forms toxic mixtures in water, dilution measures notwithstanding.

Discharge into the environment must be avoided.

Endocrine disrupting properties

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product

itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

Not regulated as a dangerous good

IMDG-Code

Not regulated as a dangerous good

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR

Not regulated as a dangerous good

Poison Inhalation Hazard : No

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
1,4-Dioxane	123-91-1	100	5000

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Acute Health Hazard
Chronic Health Hazard

SARA 313 : The following components are subject to reporting levels established by SARA Title III, Section 313:

Dichloromethane	75-09-2	>= 1 - < 5 %
1,4-Dioxane	123-91-1	>= 1 - < 5 %

US State Regulations

Massachusetts Right To Know

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Dichloromethane	75-09-2
1,4-Dioxane	123-91-1

Pennsylvania Right To Know

Dichloromethane	75-09-2
1,4-Dioxane	123-91-1

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Dichloromethane	75-09-2
1,4-Dioxane	123-91-1

Washington Chemicals of High Concern

Dichloromethane	75-09-2
1,4-Dioxane	123-91-1

California Prop. 65

WARNING: This product can expose you to chemicals including Dichloromethane, which is/are known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov. **The components of this product are reported in the following inventories:**

US TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

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The following substance(s) is/are subject to TSCA 12(b) export notification requirements:
Dichloromethane 75-09-2

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH	: USA. ACGIH Threshold Limit Values (TLV)
ACGIH BEI	: ACGIH - Biological Exposure Indices (BEI)
NIOSH REL	: USA. NIOSH Recommended Exposure Limits
OSHA CARC	: OSHA Specifically Regulated Chemicals/Carcinogens
OSHA P0	: USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)
OSHA Z-1	: USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
TSCA ECEL	: TSCA Existing Chemical Exposure Limit
ACGIH / TWA	: 8-hour, time-weighted average
NIOSH REL / C	: Ceiling value not be exceeded at any time.
OSHA CARC / PEL	: Permissible exposure limit (PEL)
OSHA CARC / STEL	: Excursion limit
OSHA P0 / TWA	: 8-hour time weighted average
OSHA Z-1 / TWA	: 8-hour time weighted average
TSCA ECEL / ECEL-TWA	: Existing Chemical Exposure List (TWA)
TSCA ECEL / EPA STEL	: EPA STEL

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and

Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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