

### 1. PRODUCT AND COMPANY 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

#### 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

#### 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

### 2. HAZARDS IDENTIFICATION

#### 2.1 Classification of the substance or mixture

##### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Carcinogenicity (Category 2), H351

Specific target organ toxicity - repeated exposure, Oral (Category 2), Liver, Blood, H373

Specific target organ toxicity - repeated exposure, Inhalation (Category 2), Central nervous system, H373

For the full text of the H-Statements mentioned in this Section, see Section 16.

#### 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word : Warning

Hazard statement(s)

H351

Suspected of causing cancer.

H373

May cause damage to organs (Liver, Blood) through prolonged or repeated exposure if swallowed.

H373

May cause damage to organs (Central nervous system) through prolonged or repeated exposure if inhaled.

Precautionary statement(s)

P201

Obtain special instructions before use.

P202

Do not handle until all safety precautions have been read and understood.

P260

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

P280

Wear protective gloves/ protective clothing/ eye protection/ face

P308 + P313	protection.
P405	IF exposed or concerned: Get medical advice/ attention.
P501	Store locked up.
	Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Synonyms : *cis*-Propene-1,2,3-tricarboxylic acid

Formula : C<sub>6</sub>H<sub>6</sub>O<sub>6</sub>

Molecular weight : 174.11 g/mol

CAS-No. : 585-84-2

#### Hazardous components

Component	Classification	Concentration
<b>Methylene chloride</b>		
	Skin Irrit. 2; Eye Irrit. 2A; Carc. 2; STOT SE 3; STOT RE 2; H315, H319, H335, H336, H351, H373, H373	>= 1 - < 5 %
<b>1,4-Dioxane</b>		
	Flam. Liq. 2; Eye Irrit. 2A; Carc. 2; STOT SE 3; H225, H319, H335, H351	>= 1 - < 5 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

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

### 5.2 Special hazards arising from the substance or mixture

No data available

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

No data available

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## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.  
For personal protection see section 8.

### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

### 6.4 Reference to other sections

For disposal see section 13.

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## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.  
Provide appropriate exhaust ventilation at places where dust is formed.  
For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Recommended storage temperature -20 °C

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
	Remarks	Potential Occupational Carcinogen See Appendix A		
Methylene chloride	75-09-2	TWA	50.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Carboxyhemoglobinemia Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Confirmed animal carcinogen with unknown relevance to humans		
		TWA	50 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Carboxyhemoglobinemia Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Confirmed animal carcinogen with unknown relevance to humans		
		Substance listed; for more information see OSHA document 1910.1052		
		Substance listed; for more information see OSHA document 1910.1052		

		See Table Z-2		
		PEL	25.000000 ppm	OSHA Specifically Regulated Chemicals/Carcinogens
		1910.1052 This section applies to all occupational exposures to methylene chloride (MC), Chemical Abstracts Service Registry Number 75-09-2, in general industry, construction and shipyard employment. Methylene chloride (MC) means an organic compound with chemical formula, CH <sub>2</sub> Cl <sub>2</sub> . Its Chemical Abstracts Service Registry Number is 75-09-2. Its molecular weight is 84.9 g/mole OSHA specifically regulated carcinogen		
		STEL	125.000000 ppm	OSHA Specifically Regulated Chemicals/Carcinogens
		1910.1052 This section applies to all occupational exposures to methylene chloride (MC), Chemical Abstracts Service Registry Number 75-09-2, in general industry, construction and shipyard employment. Methylene chloride (MC) means an organic compound with chemical formula, CH <sub>2</sub> Cl <sub>2</sub> . Its Chemical Abstracts Service Registry Number is 75-09-2. Its molecular weight is 84.9 g/mole OSHA specifically regulated carcinogen		
		PEL	25 ppm 87 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		see section 5202		
		STEL	125 ppm 435 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		see section 5202		
1,4-Dioxane	123-91-1	TWA	20.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Liver damage Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Liver damage Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		TWA	25 ppm 90 mg/m <sup>3</sup>	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		TWA	100.000000 ppm 360.000000 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation The value in mg/m <sup>3</sup> is approximate.		
		TWA	100 ppm 360 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation The value in mg/m <sup>3</sup> is approximate.		
		C	1.000000 ppm 3.600000 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		Potential Occupational Carcinogen See Appendix A		

		30 minute ceiling value		
		PEL	0.28 ppm 1 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

#### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Methylene chloride	75-09-2	Dichloromethane	0.3000 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			

## 8.2 Exposure controls

### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

### Personal protective equipment

#### Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

#### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

#### Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

#### Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

#### Body Protection

Impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: solid
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 122 °C (252 °F) - lit.
f) Initial boiling point and boiling range	No data available
g) Flash point	No data available
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapour pressure	No data available
l) Vapour density	No data available
m) Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Auto-ignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

### 9.2 Other safety information

No data available

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

No data available

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen chloride gas  
Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

IARC: 2B - Group 2B: Possibly carcinogenic to humans (1,4-Dioxane)

NTP: Reasonably anticipated to be a human carcinogen (1,4-Dioxane)

OSHA: OSHA specifically regulated carcinogen (Methylene chloride)

#### Reproductive toxicity

No data available

No data available

#### Specific target organ toxicity - single exposure

No data available

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

No data available

#### Additional Information

RTECS: Not available

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence (Methylene chloride)

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## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

No data available

### 12.2 Persistence and degradability

No data available

### 12.3 Bioaccumulative potential

No data available

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

### 12.6 Other adverse effects

No data available

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### 13. DISPOSAL CONSIDERATIONS

#### 13.1 Waste treatment methods

##### Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

##### Contaminated packaging

Dispose of as unused product.

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### 14. TRANSPORT INFORMATION

#### DOT (US)

Not dangerous goods

#### IMDG

Not dangerous goods

#### IATA

Not dangerous goods

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### 15. REGULATORY INFORMATION

#### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

#### SARA 313 Components

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

	CAS-No.	Revision Date
1,4-Dioxane	123-91-1	2007-07-01

#### SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

#### Massachusetts Right To Know Components

	CAS-No.	Revision Date
Methylene chloride	75-09-2	2007-07-01
1,4-Dioxane	123-91-1	2007-07-01

#### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
cis-Aconitic acid	585-84-2	
Methylene chloride	75-09-2	2007-07-01
1,4-Dioxane	123-91-1	2007-07-01

#### New Jersey Right To Know Components

	CAS-No.	Revision Date
cis-Aconitic acid	585-84-2	
Methylene chloride	75-09-2	2007-07-01
1,4-Dioxane	123-91-1	2007-07-01

#### California Prop. 65 Components

WARNING! This product contains a chemical known to the State of California to cause cancer.

	CAS-No.	Revision Date
Methylene chloride	75-09-2	2007-09-28
1,4-Dioxane	123-91-1	2007-09-28



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## 16. OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3.

Carc.	Carcinogenicity
Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
H351	Suspected of causing cancer.
H373	May cause damage to organs (/\$/*_2ORG_REP_INH\$/) through prolonged or repeated exposure if inhaled.
Skin Irrit.	Skin irritation
STOT RE	Specific target organ toxicity - repeated exposure
STOT SE	Specific target organ toxicity - single exposure

### HMIS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	0
Physical Hazard	0

### NFPA Rating

Health hazard:	2
Fire Hazard:	0
Reactivity Hazard:	0

### Further information

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### Preparation Information

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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