

SAFETY DATA SHEET

Version 6.8
Revision Date 09/08/2024
Print Date 09/09/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Crotyl chloride

Product Number : 28115
Brand : Aldrich
CAS-No. : 591-97-9

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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

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

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 3), H301
Skin corrosion (Category 1A), H314
Serious eye damage (Category 1), H318

Aldrich - 28115

Page 1 of 13

Skin sensitization (Category 1), H317
Short-term (acute) aquatic hazard (Category 3), H402
Long-term (chronic) aquatic hazard (Category 3), H412

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

Danger

Hazard Statements

H225	Highly flammable liquid and vapor.
H301	Toxic if swallowed.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H412	Harmful to aquatic life with long lasting effects.

Precautionary Statements

P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P272	Contaminated work clothing must not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Lachrymator.

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Synonyms : cis,trans-1-Chloro-2-butene

Molecular weight : 90.55 g/mol

Component		Classification	Concentration
1-chloro-2-butene (mixture of cis/trans isomers)			
CAS-No.	591-97-9	Flam. Liq. 2; Acute Tox. 3; Acute Tox. 4; Skin Corr. 1A; Eye Dam. 1; Skin Sens. 1; Aquatic Acute 3; Aquatic Chronic 3; H225, H301, H332, H314, H318, H317, H402, H412	>= 70 - < 90 %
EC-No.	209-739-5		
3-Chlorobut-1-ene			
CAS-No.	563-52-0	Flam. Liq. 2; Skin Sens. 1; H225, H317	>= 30 - < 50 %
EC-No.	209-252-8		

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

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

First aiders need to protect themselves. Show this material 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. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal

(20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible. Do not attempt to neutralise.

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Hydrogen chloride gas

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 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 with liquid-absorbent material (e.g.

Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

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.

Splash contact

Material: Fluorinated rubber

Minimum layer thickness: 0.7 mm

Break through time: 120 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, 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 EC 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

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter type ABEK

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.

required when vapours/aerosols 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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|--|--|
| a) Appearance | Form: clear, liquid
Color: colorless |
| b) Odor | pungent |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/ range: -65 °C (-85 °F) |
| f) Initial boiling point and boiling range | 85 - 86 °C 185 - 187 °F - lit. |
| g) Flash point | -12 °C (10 °F) - closed cup - DIN 51755 Part 1 |
| h) Evaporation rate | No data available |

i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	116 hPa at 20 °C (68 °F)
l) Vapor density	No data available
m) Density	0.923 g/mL at 20 °C (68 °F) - lit.
Relative density	No data available
n) Water solubility	ca.14 g/l at 20 °C (68 °F) - hydrolyzes
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	Not classified as explosive.
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Acute toxicity estimate Oral - 142.86 mg/kg

(Calculation method)

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

Acute toxicity estimate Inhalation - 4 h - 23.29 mg/l - vapor (Calculation method)

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages: damage of respiratory tract

Dermal: No data available

No data available

Skin corrosion/irritation

Remarks: Mixture causes severe burns.

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye damage.

Risk of blindness!

Respiratory or skin sensitization

Mixture may cause an allergic skin reaction.

Germ cell mutagenicity

No data available

Test Type: Ames test

Test system: *S. typhimurium*

Result: positive

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

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

11.2 Additional Information

RTECS: EM4264000

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea
Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Components

1-chloro-2-butene (mixture of cis/trans isomers)

Acute toxicity

LD50 Oral - Rat - 172 - 219 mg/kg
(OECD Test Guideline 401)

Symptoms: After swallowing: burns in mouth, throat, oesophagus and gastrointestinal tract.

Oral: absorption

LC50 Inhalation - Rat - 4 h - 16.3 mg/l - vapor

Remarks: (External MSDS)

Symptoms: Shortness of breath, Cough, mucosal irritations, Possible damages:, damage of respiratory tract

Inhalation: absorption

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Causes burns.

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: slight irritation

(OECD Test Guideline 405)

Remarks: Causes serious eye damage.

Respiratory or skin sensitization

Sensitisation test: - Guinea pig

Result: positive

Remarks: (Lit.)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Result: positive

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Acute oral toxicity - After swallowing: burns in mouth, throat, oesophagus and gastrointestinal tract.

Acute inhalation toxicity - Shortness of breath, Cough, mucosal irritations, Possible damages:, damage of respiratory tract

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

3-Chlorobut-1-ene**Acute toxicity**

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: 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

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

SECTION 12: Ecological information**12.1 Toxicity****Mixture**

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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Components

1-chloro-2-butene (mixture of cis/trans isomers)

Toxicity to daphnia
and other aquatic
invertebrates

EC50 - Daphnia magna (Water flea) - 42 mg/l - 48 h
Remarks: (External MSDS)

3-Chlorobut-1-ene

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

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

DOT (US)

UN number: 2920 Class: 8 (3)

Packing group: I

Proper shipping name: Corrosive liquids, flammable, n.o.s. (1-chloro-2-butene (mixture of cis/trans isomers), 3-Chlorobut-1-ene)

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG

UN number: 2920 Class: 8 (3) Packing group: I EMS-No: F-E, S-C
Proper shipping name: CORROSIVE LIQUID, FLAMMABLE, N.O.S. (1-chloro-2-butene (mixture of cis/trans isomers), 3-Chlorobut-1-ene)

IATA

UN number: 2920 Class: 8 (3) Packing group: I
Proper shipping name: Corrosive liquid, flammable, n.o.s. (1-chloro-2-butene (mixture of cis/trans isomers), 3-Chlorobut-1-ene)

SECTION 15: Regulatory information**CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

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 : Fire Hazard
Acute Health Hazard
Chronic Health Hazard

SARA 313 : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

US State Regulations**Massachusetts Right To Know**

1-chloro-2-butene (mixture of cis/trans isomers) 591-97-9

Pennsylvania Right To Know

1-chloro-2-butene (mixture of cis/trans isomers) 591-97-9

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

Further information

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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 6.8

Revision Date: 09/08/2024

Print Date: 09/09/2024