

## SAFETY DATA SHEET

Version 6.7  
Revision Date 03/29/2022  
Print Date 05/28/2022

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

Product name : Hexachloro-1,3-butadiene

Product Number : 112194  
Brand : Aldrich  
CAS-No. : 87-68-3

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

Identified uses : Research and development as defined in 40 C.F.R. § 751.403.  
See section 15 for more information.  
Uses advised against : For R&D use only. Not for pharmaceutical, household or other uses.

**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)**

Acute toxicity, Oral (Category 3), H301  
Acute toxicity, Dermal (Category 2), H310  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Carcinogenicity (Category 2), H351  
Short-term (acute) aquatic hazard (Category 1), H400  
Long-term (chronic) aquatic hazard (Category 1), H410

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 statement(s)

H301 Toxic if swallowed.  
H310 Fatal in contact with skin.  
H315 Causes skin irritation.  
H319 Causes serious eye irritation.  
H351 Suspected of causing cancer.  
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P201 Obtain special instructions before use.  
P202 Do not handle until all safety precautions have been read and understood.  
P262 Do not get in eyes, on skin, or on clothing.  
P264 Wash skin thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
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.  
P302 + P350 + P310 IF ON SKIN: Gently wash with plenty of soap and water. Immediately call a POISON CENTER or doctor/ physician.  
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.  
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.  
P391 Collect spillage.  
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 - none

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : Perchlorobutadiene  
Formula : C<sub>4</sub>Cl<sub>6</sub>  
Molecular weight : 260.76 g/mol  
CAS-No. : 87-68-3  
EC-No. : 201-765-5

Component	Classification	Concentration
-----------	----------------	---------------

<b>Hexachlorobuta-1,3-diene</b>		
	Acute Tox. 3; Acute Tox. 2; Skin Irrit. 2; Eye Irrit. 2A; Carc. 2; Aquatic Acute 1; Aquatic Chronic 1; H301, H310, H315, H319, H351, H400, H410	<= 100 %

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. 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.

### 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

Water 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.

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

### **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**

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. 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.

### **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 safe handling**

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

#### **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**

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

#### **Storage class**

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

### **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

Component	CAS-No.	Value	Control parameters	Basis
Hexachlorobuta-1,3-diene	87-68-3	TWA	0.02 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		TWA	0.02 ppm 0.24 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential Occupational Carcinogen Potential for dermal absorption		
		TWA	0.02 ppm 0.24 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		PEL	0.02 ppm 0.24 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

### 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). Safety glasses

##### Body Protection

protective clothing

##### Respiratory protection

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.

---

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- a) Appearance                      Form: liquid, clear  
   Color: light yellow

Aldrich - 112194

Page 5 of 10

b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: -22 - -19 °C (-8 - -2 °F) - lit.
f) Initial boiling point and boiling range	210 - 220 °C 410 - 428 °F - lit.
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) Vapor pressure	0.3 hPa at 20.0 °C (68.0 °F)
l) Vapor density	No data available
m) Density	1.665 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	No data available
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	No data available
t) Oxidizing properties	No data available

## 9.2 Other safety information

No data available

---

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 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

no information available

## 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

#### Acute toxicity

LD50 Oral - Rat - 82.0 mg/kg

LC50 Inhalation - Mouse - 370.0 mg/m<sup>3</sup> - dust/mist

LD50 Dermal - Rabbit - 100.0 mg/kg

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 24 h

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Mild eye irritation

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

This product is or contains a component that has been reported to be possibly carcinogenic based on its IARC, ACGIH, NTP, or EPA classification.

Suspected of causing cancer.

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: EJ0700000

Liver injury may occur., Kidney injury may occur., 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, Vomiting

Liver -

---

## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 0.09 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia - 0.5 mg/l - 24 h

### 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

---

## 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. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

---

## SECTION 14: Transport information

### DOT (US)

UN number: 2279	Class: 6.1	Packing group: III
Proper shipping name: Hexachlorobutadiene		
Reportable Quantity (RQ): 1 lbs		
Reportable Quantity (RQ): 1 lbs		
Poison Inhalation Hazard: No		

Aldrich - 112194

Page 8 of 10



**IMDG**

UN number: 2279    Class: 6.1    Packing group: III    EMS-No: F-A, S-A  
Proper shipping name: HEXACHLOROBUTADIENE  
Marine pollutant : yes

**IATA**

UN number: 2279    Class: 6.1    Packing group: III  
Proper shipping name: Hexachlorobutadiene

---

**SECTION 15: Regulatory information****US TSCA Section 3**

This chemical/product is not and cannot be distributed in commerce (as defined in TSCA section 3(5)) or processed (as defined in TSCA section 3(13)) for consumer paint or coating removal.

**SARA 302 Components**

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

**SARA 313 Components**

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

	CAS-No.	Revision Date
Hexachlorobuta-1,3-diene	87-68-3	2020-07-14

**SARA 311/312 Hazards**

Acute Health Hazard

**Reportable Quantity** : D033 lbs

**Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

**Other regulations**

This material is or contains a chemical identified as a Persistent Bioaccumulative and Toxic Chemical under 40 C.F.R. §751 Subpart E. MilliporeSigma is supplying this chemical in compliance with 40 C.F.R. § 751.401. It may only be used for research and development as defined in 40 C.F.R. § 751.403, specifically, it may only be used "for purposes of scientific experimentation or analysis, or chemical research on, or analysis of, the chemical substance, including methods for disposal, but not for research or analysis for the development of a new product, or refinement of an existing product that contains the chemical substance.

---

## SECTION 16: Other information

### Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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](http://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](mailto:mlsbranding@sial.com).

Version: 6.7

Revision Date: 03/29/2022

Print Date: 05/28/2022