

## Chemical Safety Data Sheet MSDS / SDS

## Hexachloro-1,3-butadiene

Revision Date:2025-03-01 Revision Number:1

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

## Product identifier

Product name : Hexachloro-1,3-butadiene  
CBnumber : CB6854522  
CAS : 87-68-3  
EINECS Number : 201-765-5  
Synonyms : Hexachlorobutadiene,Hexachloro-1,3-butadiene

## 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 : 010-86108875

## SECTION 2: Hazards identification

## GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

## Precautionary statements

P405 Store locked up.

P330 Rinse mouth.

P320 Specific treatment is urgent (see ... on this label).

P311 Call a POISON CENTER or doctor/physician.

P310 Immediately call a POISON CENTER or doctor/physician.

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

Continuerinsing.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

P302+P350 IF ON SKIN: Gently wash with plenty of soap and water.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

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

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

#### **Hazard statements**

H410 Very toxic to aquatic life with long lasting effects

H400 Very toxic to aquatic life

H370 Causes damage to organs

H361 Suspected of damaging fertility or the unborn child

H351 Suspected of causing cancer

H331 Toxic if inhaled

H330 Fatal if inhaled

H319 Causes serious eye irritation

H318 Causes serious eye damage

H315 Causes skin irritation

H311 Toxic in contact with skin

H310 Fatal in contact with skin

H301 Toxic if swallowed

H225 Highly Flammable liquid and vapour

#### **Disposal**

WARNING.Cancer - <https://oehha.ca.gov/proposition-65/chemicals/hexachlorobutadiene>

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: Hexachloro-1,3-butadiene
Synonyms	: Hexachlorobutadiene,Hexachloro-1,3-butadiene
CAS	: 87-68-3
EC number	: 201-765-5
MF	: C4Cl6
MW	: 260.76

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## SECTION 4: First aid measures

### **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.

### 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

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

No data available

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

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

### 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.

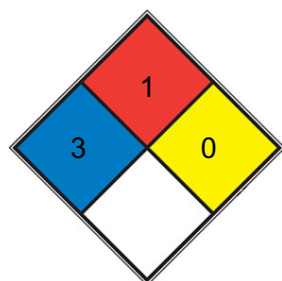
### Advice for firefighters

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

### 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.

### NFPA 704



■ HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

■ FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

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☐ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

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☐ SPEC.

☐ HAZ.

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## SECTION 6: Accidental release measures

### 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.

### 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 with liquid-absorbent material (e.g.

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

### Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 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.

### 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.

#### Specific end use(s)

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

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## SECTION 8: Exposure controls/personal protection

### control parameter

#### Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

### Exposure controls

#### 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

##### 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.

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.

#### Control of environmental exposure

Do not let product enter drains.

#### Exposure limits

Potential occupational carcinogen. NIOSH REL: TWA 20 ppb (240 mg/m<sup>3</sup>); ACGIH TLV: TWA 0.02 ppm (adopted).

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	light yellow liquid, clear
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: -22 - -19 °C - lit.
Initial boiling point and boiling range	210 - 220 °C - lit.
Flash point	210-220°C
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	0,3 hPa at 20,0 °C
Vapour density	No data available

Relative density	No data available
Water solubility	Soluble in ethanol and ether (U.S. EPA, 1985)
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available
Henry's Law Constant	3.55, 5.87, 6.90, 10.5, and 15.3 at 2.0, 6.0, 10.0, 18.0, and 25.0 °C, respectively (EPICS-SPME, Dewulf et al., 1999)

### Other safety information

No data available

## SECTION 10: Stability and reactivity

### Reactivity

No data available

### Chemical stability

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

### Possibility of hazardous reactions

No data available

### Conditions to avoid

no information available

### Incompatible materials

Strong oxidizing agents

### Hazardous decomposition products

In the event of fire: see section 5

## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 82,0 mg/kg

LC50 Inhalation - Mouse - 370,0 mg/m3

LD50 Dermal - Rabbit - 100,0 mg/kg

#### 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**

No data available

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure Aspiration hazard**

No data available

**Toxicity**

LD50 in male, female mice, rats (mg/kg): 105, 76, 216, 175 i.p.; 80, 65, 250, 270 orally (Gradiski)

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## SECTION 12: Ecological information

### 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

### Persistence and degradability

No data available

### Bioaccumulative potential

No data available

### Mobility in soil

No data available

### Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

### Toxics Screening Level

The Initial Risk Screening Level (IRSL) for hexachlorobutadiene is 0.05 µg/m<sup>3</sup> based on an annual averaging time.

## Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### Waste treatment methods

#### Product

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.

#### Incompatibilities

Strong reaction with oxidizers, aluminum powder. Attacks aluminum; some plastics, rubber and coatings

#### Waste Disposal

High temperature incineration with flue gas scrubbing. Consult with environmental regulatory agencies for guidance on acceptable disposal practices. Generators of waste containing this contaminant ( $\geq 100$  kg/mo) must conform to EPA regulations governing storage, transportation, treatment, and waste disposal.

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## SECTION 14: Transport information

### UN number

ADR/RID: 2279 IMDG: 2279 IATA: 2279

### UN proper shipping name

	ADR/RID: HEXACHLOROBUTADIENE IMDG: HEXACHLOROBUTADIENE	
	IATA: Hexachlorobutadiene	
14.3	Transport hazard class(es)	
	ADR/RID: 6.1 IMDG: 6.1	IATA: 6.1
14.4	Packaging group	
	ADR/RID: III IMDG: III	IATA: III
14.5	Environmental hazards	
	ADR/RID: no IMDG Marine pollutant: yes	IATA: no
14.6	Special precautions for user	
	No data available	

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## SECTION 15: Regulatory information

### Safety, health and environmental regulations/legislation specific for the substance or mixture

#### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015: Listed. website: <https://www.mem.gov.cn/>

#### Measures for Environmental Management of New Chemical Substances



Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

EC Inventory:Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

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## SECTION 16: Other information

### Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

ATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

### References

【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:  
[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)

【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

### Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.