

• SAFETY DATA SHEET

Version 8.11
Revision Date 11/06/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Hexachloro-1,3-butadiene

Product Number : 48543
Brand : Supelco
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.

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 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

Acute toxicity (Oral) : Category 3

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Acute toxicity (Dermal) : Category 2

Skin irritation : Category 2

Eye irritation : Category 2A

Carcinogenicity : Category 2

Short-term (acute) aquatic hazard : Category 1

Long-term (chronic) aquatic hazard : Category 1

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : 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 statements : **Prevention:**
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.

Response:
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.

Storage:

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. : 87-68-3

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Hexachlorobuta-1,3-diene	87-68-3*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : First aiders need to protect themselves.
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.
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.
- 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
- 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 (CO₂)
Dry powder
- Unsuitable extinguishing media : For this substance/mixture no limitations of extinguishing agents are given.
- Specific hazards during fire fighting : Combustible.

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

- Hazardous combustion products : Carbon oxides

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:
Do not breathe vapours, aerosols.
Avoid substance contact.
Ensure adequate ventilation.
Evacuate the danger area, observe emergency procedures, consult an expert.
Advice for emergency responders:
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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on safe handling : Work under hood. Do not inhale substance/mixture.
Avoid generation of vapours/aerosols.

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

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

Recommended storage temperature : Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
Hexachlorobuta-1,3-diene	87-68-3	TWA	0.02 ppm	ACGIH
		TWA	0.02 ppm 0.24 mg/m3	NIOSH REL

Engineering measures : No data available

Personal protective equipment

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.

Hand protection

Remarks : required

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 : liquid

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Color	: light yellow
Odor	: No data available
Odor Threshold	: No data available
pH	: No data available
Melting point/ range	: -8 °F / -22 °C
Boiling point/boiling range	: 410 - 428 °F / 210 - 220 °C Method: lit.
Flash point	: No data available
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
Vapor pressure	: 0.3 hPa (68.0 °F / 20.0 °C)
Relative vapour density	: No data available
Relative density	: No data available
Density	: 1.665 g/cm ³ (77 °F / 25 °C) Method: lit.
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

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Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Molecular weight	: 260.76 g/mol
Particle characteristics	
Particle size	: 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

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 82.0 mg/kg

LC50 Inhalation - Mouse - 370.0 mg/m³ - 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

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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 component 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 component 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**Ecotoxicity****Components:****Hexachlorobuta-1,3-diene:**

Toxicity to fish : LC50 (Pimephales promelas (fathead minnow)): 0.09 mg/l
End point: mortality
Exposure time: 96 h

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia (water flea)): 0.5 mg/l
Exposure time: 24 h

Toxicity to fish (Chronic toxicity) : LOEC (Pimephales promelas (fathead minnow)):
0.013 mg/l
Exposure time: 28 d

Ecotoxicology Assessment

Acute aquatic toxicity : Very toxic to aquatic life.

Chronic aquatic toxicity : Very toxic to aquatic life with long lasting effects.

Persistence and degradability

Components:

Hexachlorobuta-1,3-diene:

Biodegradability : Remarks: No data available

Bioaccumulative potential

Components:

Hexachlorobuta-1,3-diene:

Bioaccumulation : Remarks: No data available

Mobility in soil

Components:

Hexachlorobuta-1,3-diene:

Stability in soil : Remarks: No data available

Other adverse effects

Components:

Hexachlorobuta-1,3-diene:

Results of PBT and vPvB assessment : PBT substance

Additional ecological information : 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

UN/ID No. : UN 2279
Proper shipping name : Hexachlorobutadiene
Class : 6.1
Packing group : III
Labels : Division 6.1 - Toxic substances
Packing instruction (cargo aircraft) : 663
Packing instruction (passenger aircraft) : 655

IMDG-Code

UN number : UN 2279
Proper shipping name : HEXACHLOROBUTADIENE

Class : 6.1
Packing group : III
Labels : 6.1
EmS Code : F-A, S-A
Marine pollutant : yes

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number : UN 2279
Proper shipping name : Hexachlorobutadiene

Class : 6.1
Packing group : III
Labels : Division 6.1 - Toxic substances
ERG Code : 151
Marine pollutant : yes

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

Components	CAS-No.	Component	Calculated product
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		RQ (lbs)	RQ (lbs)
Hexachlorobuta-1,3-diene	87-68-3	1	1
Hexachlorobuta-1,3-diene	87-68-3	1	1 (D033)

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

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

Hexachlorobut a-1,3-diene 87-68-3 >= 90 - <= 100 %

US State Regulations

Massachusetts Right To Know

Hexachlorobuta-1,3-diene 87-68-3

Pennsylvania Right To Know

Hexachlorobuta-1,3-diene 87-68-3

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Hexachlorobuta-1,3-diene 87-68-3

Washington Chemicals of High Concern

Hexachlorobuta-1,3-diene 87-68-3

California Prop. 65

WARNING: This product can expose you to chemicals including Hexachlorobuta-1,3-diene, which is/are known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov.

International Regulations

Stockholm Convention (Persistent Organic Pollutants) : Hexachlorobuta-1,3-diene

The components 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.

The following substance(s) is/are subject to TSCA 12(b) export notification requirements:

SECTION 16. OTHER INFORMATION**Full text of other abbreviations**

ACGIH	: USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL	: USA. NIOSH Recommended Exposure Limits
ACGIH / TWA	: 8-hour, time-weighted average
NIOSH REL / TWA	: Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek

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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