

### SECTION 1: Identification

#### 1.1. Identification

Product form	: Substance
Substance name	: Hexachloro-1,3-butadiene
CAS No	: 87-68-3
Product code	: 1300-4-04
Formula	: C4Cl6
Synonyms	: Perchlorobutadiene
Other means of identification	: MFCD00000836

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

Use of the substance/mixture	: Laboratory chemicals Manufacture of substances Scientific research and development
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#### 1.3. Details of the supplier of the safety data sheet

SynQuest Laboratories, Inc.  
P.O. Box 309  
Alachua, FL 32615 - United States of America  
T (386) 462-0788 - F (386) 462-7097  
[info@synquestlabs.com](mailto:info@synquestlabs.com) - [www.synquestlabs.com](http://www.synquestlabs.com)

#### 1.4. Emergency telephone number

Emergency number : (844) 523-4086 (3E Company - Account 10069)

### SECTION 2: Hazard(s) identification

#### 2.1. Classification of the substance or mixture

##### Classification (GHS-US)

Acute Tox. 2 (Oral)	H300 - Fatal if swallowed
Acute Tox. 4 (Dermal)	H312 - Harmful in contact with skin
Skin Irrit. 2	H315 - Causes skin irritation
Eye Dam. 1	H318 - Causes serious eye damage
Carc. 2	H351 - Suspected of causing cancer
STOT SE 3	H335 - May cause respiratory irritation
Aquatic Acute 1	H400 - Very toxic to aquatic life
Aquatic Chronic 1	H410 - Very toxic to aquatic life with long lasting effects

Full text of H-phrases: see section 16

#### 2.2. Label elements

##### GHS-US labeling

Hazard pictograms (GHS-US) :



Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H300 - Fatal if swallowed  
H312 - Harmful in contact with skin  
H315 - Causes skin irritation  
H318 - Causes serious eye damage  
H335 - May cause respiratory irritation  
H351 - Suspected of causing cancer  
H410 - Very toxic to aquatic life with long lasting effects

Precautionary statements (GHS-US) :

P201 - Obtain special instructions before use  
P202 - Do not handle until all safety precautions have been read and understood  
P261 - Avoid breathing fumes, mist, spray, vapors  
P264 - Wash skin thoroughly after handling  
P270 - Do not eat, drink or smoke when using this product  
P271 - Use only outdoors or in a well-ventilated area  
P273 - Avoid release to the environment

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P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P301+P310 - If swallowed: Immediately call a poison center/doctor/...  
P302+P352 - If on skin: Wash with plenty of soap and water  
P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing  
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  
P310 - Immediately call a POISON CENTER or doctor/ physician  
P321 - Specific treatment (see supplemental first aid instructions on this label)  
P330 - Rinse mouth  
P332+P313 - If skin irritation occurs: Get medical advice/attention  
P362+P364 - Take off contaminated clothing and wash it before reuse  
P391 - Collect spillage  
P403+P233 - Store in a well-ventilated place. Keep container tightly closed  
P405 - Store locked up  
P501 - Dispose of contents/container to an approved waste disposal plant

### 2.3. Other hazards

No additional information available

### 2.4. Unknown acute toxicity (GHS US)

Not applicable

## SECTION 3: Composition/information on ingredients

### 3.1. Substance

Substance type : Mono-constituent

Name	Product identifier	%	Classification (GHS-US)
Hexachloro-1,3-butadiene (Main constituent)	(CAS No) 87-68-3	<= 100	Acute Tox. 2 (Oral), H300 Acute Tox. 4 (Dermal), H312 Skin Irrit. 2, H315 Eye Dam. 1, H318 Carc. 2, H351 STOT SE 3, H335 Aquatic Acute 1, H400 Aquatic Chronic 1, H410

Full text of H-phrases: see section 16

### 3.2. Mixture

Not applicable

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

First-aid measures general : In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Move the affected personnel away from the contaminated area.

First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing. If not breathing, give artificial respiration. Get immediate medical advice/attention.

First-aid measures after skin contact : Wash with plenty of soap and water. Remove contaminated clothing and shoes. Get immediate medical advice/attention.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get immediate medical advice/attention.

First-aid measures after ingestion : Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get immediate medical advice/attention.

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

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

Symptoms/injuries after inhalation : Material is destructive to tissue of the mucuous membranes and upper respiratory tract. Cough, shortness of breath, headache, nausea.

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

Treat symptomatically.

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

Suitable extinguishing media : Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media appropriate for surrounding fire.

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

- Fire hazard : Thermal decomposition generates: Carbon oxides. Hydrogen chloride.
- Explosion hazard : Risk of explosion if heated under confinement. Use water spray or fog for cooling exposed containers.

### 5.3. Advice for firefighters

- Firefighting instructions : In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.
- Protection during firefighting : Wear gas tight chemically protective clothing in combination with self contained breathing apparatus. For further information refer to section 8: "Exposure controls/personal protection".

## SECTION 6: Accidental release measures

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

- General measures : Evacuate unnecessary personnel. Ensure adequate air ventilation. Do not breathe gas, fumes, vapor or spray.

#### 6.1.1. For non-emergency personnel

- Emergency procedures : Only qualified personnel equipped with suitable protective equipment may intervene.

#### 6.1.2. For emergency responders

- Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".
- Emergency procedures : Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level.

### 6.2. Environmental precautions

Avoid release to the environment. Notify authorities if product enters sewers or public waters.

### 6.3. Methods and material for containment and cleaning up

- For containment : Stop leak if safe to do so. Dike for recovery or absorb with appropriate material.
- Methods for cleaning up : Take up large spills with pump or vacuum and finish with dry chemical absorbent. Use explosion-proof equipment. Take up small spills with dry chemical absorbent. Sweep or shovel spills into appropriate container for disposal. Ventilate area.
- Other information : For disposal of solid materials or residues refer to section 13 : "Disposal considerations".

### 6.4. Reference to other sections

No additional information available

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

- Precautions for safe handling : Do not handle until all safety precautions have been read and understood. Ensure good ventilation of the work station. Do not breathe fumes, mist, spray, vapors. Wear personal protective equipment. Avoid contact with skin and eyes.
- Hygiene measures : Handle in accordance with good industrial hygiene and safety procedures. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

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

- Technical measures : Comply with applicable regulations.
- Storage conditions : Keep container closed when not in use.
- Incompatible materials : Refer to Section 10 on Incompatible Materials.
- Storage area : Store in dry, cool, well-ventilated area.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

Hexachloro-1,3-butadiene (87-68-3)		
ACGIH	ACGIH TWA (ppm)	0.02 ppm
ACGIH	Remark (ACGIH)	Kidney dam

### 8.2. Exposure controls

- Appropriate engineering controls : Ensure good ventilation of the work station. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.
- Hand protection : Protective gloves. 29 CFR 1910.138: Hand Protection.

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Eye protection	: Chemical goggles or safety glasses. Face shield. 29 CFR 1910.133: Eye and Face Protection.
Skin and body protection	: Wear suitable protective clothing.
Respiratory protection	: In case of inadequate ventilation wear respiratory protection. 29 CFR 1910.134: Respiratory Protection.
Other information	: Safety shoes. 29 CFR 1910.136: Foot Protection.

### SECTION 9: Physical and chemical properties

#### 9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Color	: No data available
Odor	: No data available
Odor threshold	: No data available
pH	: No data available
Melting point	: -22 - -19 °C
Freezing point	: No data available
Boiling point	: 210 - 220 °C
Flash point	: No data available
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: No data available
Explosion limits	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Vapor pressure	: 0.2 mm Hg (@ 20 °C)
Relative density	: No data available
Relative vapor density at 20 °C	: No data available
Specific gravity / density	: 1.665 g/ml (@ 25 °C)
Molecular mass	: 260.76 g/mol
Solubility	: Water: 4 mg/l (at 20 °C)
Log Pow	: 4.9 (at 21.5 °C)
Auto-ignition temperature	: 610 °C
Decomposition temperature	: No data available
Viscosity	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available

#### 9.2. Other information

Refractive index	: 1.555 (@ 20 °C)
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### SECTION 10: Stability and reactivity

#### 10.1. Reactivity

No additional information available

#### 10.2. Chemical stability

The product is stable at normal handling and storage conditions.

#### 10.3. Possibility of hazardous reactions

No additional information available

#### 10.4. Conditions to avoid

Keep away from heat, sparks and flame.

#### 10.5. Incompatible materials

Strong oxidizing agents.

#### 10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced. Hazardous decomposition products in case of fire, see Section 5.

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### SECTION 11: Toxicological information

#### 11.1. Information on toxicological effects

Acute toxicity : Oral: Fatal if swallowed. Dermal: Harmful in contact with skin.

Hexachloro-1,3-butadiene (87-68-3)	
LD50 oral rat	46 mg/kg
LD50 dermal rabbit	1120 mg/kg
ATE US (oral)	46.000 mg/kg body weight
ATE US (dermal)	1120.000 mg/kg body weight

Skin corrosion/irritation : Causes skin irritation.  
Serious eye damage/irritation : Causes serious eye damage.  
Respiratory or skin sensitization : Not classified  
Germ cell mutagenicity : Not classified  
Carcinogenicity : Suspected of causing cancer.

Hexachloro-1,3-butadiene (87-68-3)	
IARC group	3 - Not classifiable

Reproductive toxicity : Not classified  
Specific target organ toxicity (single exposure) : May cause respiratory irritation.  
Specific target organ toxicity (repeated exposure) : Not classified  
Aspiration hazard : Not classified  
Symptoms/injuries after inhalation : Material is destructive to tissue of the mucuous membranes and upper respiratory tract. Cough, shortness of breath, headache, nausea.

### SECTION 12: Ecological information

#### 12.1. Toxicity

Hexachloro-1,3-butadiene (87-68-3)	
LC50 fish 1	0.09 - 0.11 mg/l (Exposure time: 96 h - Species: Pimephales promelas [flow-through])
LC50 fish 2	0.312 - 0.337 mg/l (Exposure time: 96 h - Species: Lepomis macrochirus [flow-through])

#### 12.2. Persistence and degradability

No additional information available

#### 12.3. Bioaccumulative potential

Hexachloro-1,3-butadiene (87-68-3)	
Log Pow	4.9 (at 21.5 °C)

#### 12.4. Mobility in soil

No additional information available

#### 12.5. Other adverse effects

No additional information available

### SECTION 13: Disposal considerations

#### 13.1. Waste treatment methods

Regional legislation (waste) : U.S. - RCRA (Resource Conservation & Recovery Act) - Basis for Listing - Appendix VII. U.S. - RCRA (Resource Conservation & Recovery Act) - D Series Wastes - Max Conc of Contaminants for the Tox Characteristic. U.S. - RCRA (Resource Conservation & Recovery Act) - Hazardous Constituents - Appendix VIII to 40 CFR 261. U.S. - RCRA (Resource Conservation & Recovery Act) - List for Hazardous Constituents. U.S. - RCRA (Resource Conservation & Recovery Act) - Part 268 Appendix III - Halogenated Organic Compounds (HOCs). U.S. - RCRA (Resource Conservation & Recovery Act) - Phase 4 LDR Rule - Universal Treatment Standards. U.S. - RCRA (Resource Conservation & Recovery Act) - TSD Facilities Ground Water Monitoring. U.S. - RCRA (Resource Conservation & Recovery Act) - U Series Wastes - Acutely Toxic Wastes & Other Hazardous Characteristics.  
Waste treatment methods : Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.  
Waste disposal recommendations : Dispose of contents/container in accordance with licensed collector's sorting instructions.

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Additional information : Recycle the material as far as possible.

### SECTION 14: Transport information

#### Department of Transportation (DOT)

In accordance with DOT

Transport document description : UN2279 Hexachlorobutadiene, 6.1, III

UN-No.(DOT) : UN2279

Proper Shipping Name (DOT) : Hexachlorobutadiene

Transport hazard class(es) (DOT) : 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132

Hazard labels (DOT) : 6.1 - Poison



Packing group (DOT) : III - Minor Danger

Dangerous for the environment : Yes

Marine pollutant : Yes



DOT Packaging Non Bulk (49 CFR 173.xxx) : 203

DOT Packaging Bulk (49 CFR 173.xxx) : 241

DOT Special Provisions (49 CFR 172.102) : IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672).  
T4 - 2.65 178.274(d)(2) Normal..... 178.275(d)(3)  
TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling =  $97 / 1 + a (tr - tf)$  Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling.

DOT Packaging Exceptions (49 CFR 173.xxx) : 153

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 60 L

DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 220 L

DOT Vessel Stowage Location : A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.

Emergency Response Guide (ERG) Number : 151

Other information : No supplementary information available.

#### TDG

No additional information available

#### Transport by sea

UN-No. (IMDG) : 2279

Proper Shipping Name (IMDG) : HEXACHLOROBUTADIENE

Class (IMDG) : 6.1 - Toxic substances

Packing group (IMDG) : III - substances presenting low danger

#### Air transport

UN-No. (IATA) : 2279

Proper Shipping Name (IATA) : Hexachlorobutadiene

Class (IATA) : 6.1 - Toxic Substances

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Packing group (IATA)

: III - Minor Danger

### SECTION 15: Regulatory information

#### 15.1. US Federal regulations

##### Hexachloro-1,3-butadiene (87-68-3)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

Subject to reporting requirements of United States SARA Section 313

CERCLA RQ	1 lb
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SARA Section 313 - Emission Reporting	1.0 %
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All components of this product are listed, or excluded from listing, on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory

Chemical(s) subject to the reporting requirements of Section 313 or Title III of the Superfund Amendments and Reauthorization Act (SARA) of 1986 and 40 CFR Part 372.

Hexachloro-1,3-butadiene	CAS No 87-68-3	100%
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#### 15.2. International regulations

##### CANADA

##### Hexachloro-1,3-butadiene (87-68-3)

Listed on the Canadian DSL (Domestic Substances List)

WHMIS Classification	Class B Division 3 - Combustible Liquid Class D Division 1 Subdivision B - Toxic material causing immediate and serious toxic effects Class D Division 2 Subdivision B - Toxic material causing other toxic effects
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##### EU-Regulations

No additional information available

##### National regulations

##### Hexachloro-1,3-butadiene (87-68-3)

Listed on the AICS (Australian Inventory of Chemical Substances)

Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)

Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory

Listed on the Korean ECL (Existing Chemicals List)

Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)

Listed on the Canadian IDL (Ingredient Disclosure List)

Listed on INSQ (Mexican national Inventory of Chemical Substances)

Listed on the TCSI (Taiwan Chemical Substance Inventory)

#### 15.3. US State regulations

##### Hexachloro-1,3-butadiene (87-68-3)

U.S. - California - Proposition 65 - Carcinogens List	Yes
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U.S. - California - Proposition 65 - Developmental Toxicity	No
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U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
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U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
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State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) - Environmental Hazard List U.S. - Pennsylvania - RTK (Right to Know) List
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California Proposition 65 - This product contains, or may contain, trace quantities of a substance(s) known to the state of California to cause cancer and/or reproductive toxicity

### SECTION 16: Other information

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### Full text of H-phrases:

Acute Tox. 2 (Oral)	Acute toxicity (oral) Category 2
Acute Tox. 4 (Dermal)	Acute toxicity (dermal) Category 4
Aquatic Acute 1	Hazardous to the aquatic environment - Acute Hazard Category 1
Aquatic Chronic 1	Hazardous to the aquatic environment - Chronic Hazard Category 1
Carc. 2	Carcinogenicity Category 2
Eye Dam. 1	Serious eye damage/eye irritation Category 1
Skin Irrit. 2	Skin corrosion/irritation Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H300	Fatal if swallowed
H312	Harmful in contact with skin
H315	Causes skin irritation
H318	Causes serious eye damage
H335	May cause respiratory irritation
H351	Suspected of causing cancer
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects

### NFPA health hazard

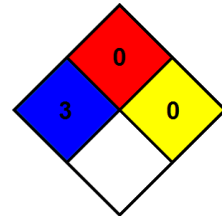
: 3 - Short exposure could cause serious temporary or residual injury even though prompt medical attention was given.

### NFPA fire hazard

: 0 - Materials that will not burn.

### NFPA reactivity

: 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



### HMIS III Rating

#### Health

: 4 Severe Hazard - Life-threatening, major or permanent damage may result from single or repeated overexposures

\* - Chronic (long-term) health effects may result from repeated overexposure

#### Flammability

: 0 Minimal Hazard - Materials that will not burn

#### Physical

: 0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

### SDS US (GHS HazCom 2012)

*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 offered solely for your consideration, investigation, and verification. It does not represent any guarantee of the properties of the product nor that the hazard precautions or procedures described are the only ones which exist. SynQuest shall not be held liable or any damage resulting from handling or from contact with the above product.*