1 Identification

Product identifier

Product name: Hexachloro-1,3-butadiene

Stock number: A17316
CAS Number:
87-68-3
EC number:
201-765-5
Relevant identified uses of the substance or mixture and uses advised against.
Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet
Manufacturer/Supplier:
Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com
Information Department: Health, Safety and Environmental Department
Emergency telephone number:
During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)

GHS06 Skull and crossbones

Acute Tox. 3 H301 Toxic if swallowed.
Acute Tox. 2 H310 Fatal in contact with skin.
Acute Tox. 2 H330 Fatal if inhaled.

GHS08 Health hazard

Carc. 2 H351 Suspected of causing cancer.
Repr. 2 H361 Suspected of damaging fertility or the unborn child.

GHS07

Skin Irrit. 2 H315 Causes skin irritation.
Eye Irrit. 2A H319 Causes serious eye irritation.
Hazards not otherwise classified No information known.

Label elements
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)
Hazard pictograms

GHS06 GHS08

Signal word Danger
Hazard statements
H301 Toxic if swallowed.
H310+H330 Fatal in contact with skin or if inhaled.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H351 Suspected of causing cancer.
H361 Suspected of damaging fertility or the unborn child.
Precautionary statements
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor/…
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P320 Specific treatment is urgent (see on this label).
P361 Take off immediately all contaminated clothing.
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.
WHMIS classification
D1A - Very toxic material causing immediate and serious toxic effects
D2A - Very toxic material causing other toxic effects

Classification system
HMIS ratings (scale 0-4)
(Hazardous Materials Identification System)

Health (acute effects) = 2
Flammability = 1
Physical Hazard = 1

(Contd. on page 2)

Product name: Hexachloro-1,3-butadiene

(Contd. of page 1)

Other hazards
Results of PBT and vPvB assessment

PBT:	
87-68-3	Hexachloro-1,3-butadiene

vPvB:	
87-68-3	Hexachloro-1,3-butadiene

3 Composition/information on ingredients

Chemical characterization: Substances
CAS# Description:
87-68-3 Hexachloro-1,3-butadiene
Identification number(s):
EC number: 201-765-5

4 First-aid measures

Description of first aid measures
General information
Immediately remove any clothing soiled by the product.
Remove breathing apparatus only after contaminated clothing has been completely removed.
In case of irregular breathing or respiratory arrest provide artificial respiration.
After inhalation
Supply fresh air. If required, provide artificial respiration. Keep patient warm.
Seek immediate medical advice.
After skin contact
Immediately wash with water and soap and rinse thoroughly.
Seek immediate medical advice.
After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.
After swallowing Do not induce vomiting; immediately call for medical help.
Information for doctor
Most important symptoms and effects, both acute and delayed No further relevant information available.
Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures

Extinguishing media
Suitable extinguishing agents Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
Special hazards arising from the substance or mixture
If this product is involved in a fire, the following can be released:
Carbon monoxide and carbon dioxide
Hydrogen chloride (HCl)
Advice for firefighters
Protective equipment:
Wear self-contained respirator.
Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures
Wear protective equipment. Keep unprotected persons away.
Ensure adequate ventilation
Environmental precautions: Do not allow product to reach sewage system or any water course.
Methods and material for containment and cleaning up:
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Dispose of contaminated material as waste according to section 13.
Ensure adequate ventilation.
Prevention of secondary hazards: No special measures required.
Reference to other sections
See Section 7 for information on safe handling
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

7 Handling and storage

Handling
Precautions for safe handling
Keep container tightly sealed.
Store in cool, dry place in tightly closed containers.
Ensure good ventilation at the workplace.
Open and handle container with care.
Information about protection against explosions and fires: No information known.

Conditions for safe storage, including any incompatibilities
Storage
Requirements to be met by storerooms and receptacles: No special requirements.
Information about storage in one common storage facility: Store away from oxidizing agents.
Further information about storage conditions:
Keep container tightly sealed.
Store in cool, dry conditions in well sealed containers.
Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:
Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Control parameters

Components with limit values that require monitoring at the workplace:	
87-68-3 Hexachloro-1,3-butadiene (100.0%)	
REL (USA)	Long-term value: 0.24 mg/m³, 0.02 ppm Skin; See Pocket Guide App. A

(Contd. on page 3)

Product name: Hexachloro-1,3-butadiene

(Contd. of page 2)

TLV (USA)	Long-term value: 0.21 mg/m³, 0.02 ppm Skin
EL (Canada)	Long-term value: 0.02 ppm Skin
EV (Canada)	Long-term value: 0.21 mg/m³, 0.02 ppm Skin

Additional information: No data

Exposure controls
Personal protective equipment
General protective and hygienic measures
The usual precautionary measures for handling chemicals should be followed.
Keep away from foodstuffs, beverages and feed.
Remove all soiled and contaminated clothing immediately.
Wash hands before breaks and at the end of work.
Store protective clothing separately.
Do not inhale dust / smoke / mist.
Avoid contact with the eyes and skin.
Maintain an ergonomically appropriate working environment.
Breathing equipment: Use self-contained respiratory protective device in emergency situations.
Recommended filter device for short term use:
Use a respirator with multi-purpose combination (US) or type ABEK (EN 14387) as a backup to engineering controls. Risk assessment should be performed to determine if air-purifying respirators are appropriate. Only use equipment tested and approved under appropriate government standards such as NIOSH (USA) or CEN (EU).
Protection of hands:
Impervious gloves
Check protective gloves prior to each use for their proper condition.
The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.
Material of gloves Nitrile rubber, NBR
Penetration time of glove material (in minutes) 480
Glove thickness 0.4 mm
Eye protection: Safety glasses
Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties
General Information
Appearance:

Form:	Liquid
Color:	Colorless to pale yellow
Odor:	Mild
Odor threshold:	Not determined.
pH-value:	Not determined.
Change in condition	
Melting point/Melting range:	-21 °C (-6 °F)
Boiling point/Boiling range:	215 °C (419 °F)
Sublimation temperature / start:	Not determined
Flammability (solid, gaseous)	Not determined.
Ignition temperature:	Not determined
Decomposition temperature:	Not determined
Auto igniting:	Not determined.
Danger of explosion:	Not determined.
Explosion limits:	
Lower:	Not determined
Upper:	Not determined
Vapor pressure at 20 °C (68 °F):	0.5 hPa
Density at 20 °C (68 °F):	1.68 g/cm³ (14.02 lbs/gal)
Relative density	Not determined.
Vapor density	Not determined.
Evaporation rate	Not determined.
Solubility in / Miscibility with	
Water at 20 °C (68 °F):	2.6 g/l
Partition coefficient (n-octanol/water):	Not determined.
Viscosity:	
dynamic:	Not determined.
kinematic:	Not determined.
Other information	No further relevant information available.

10 Stability and reactivity

Reactivity No information known.
Chemical stability Stable under recommended storage conditions.
Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.
Possibility of hazardous reactions Reacts with strong oxidizing agents
Conditions to avoid No further relevant information available.
Incompatible materials: Oxidizing agents
Hazardous decomposition products:
Carbon monoxide and carbon dioxide
Hydrogen chloride (HCl)

11 Toxicological information

Information on toxicological effects
Acute toxicity:
Fatal if inhaled.
Fatal in contact with skin.
Toxic if swallowed.
Danger through skin absorption.
The Registry of Toxic Effects of Chemical Substances (RTECS) contains acute toxicity data for this substance.

(Contd. on page 4)

Product name: Hexachloro-1,3-butadiene

(Contd. of page 3)

LD/LC50 values that are relevant for classification:

Oral	LD50	82 mg/kg (rat)
Dermal	LD50	100 mg/kg (rabbit)
Inhalative	LC50/4H	0.63 mg/l/4H (rat)

Skin irritation or corrosion: Causes skin irritation.
Eye irritation or corrosion: Causes serious eye irritation.
Sensitization: No sensitizing effects known.
Germ cell mutagenicity: The Registry of Toxic Effects of Chemical Substances (RTECS) contains mutation data for this substance.
Carcinogenicity:
Suspected of causing cancer.
ACGIH A3: Animal carcinogen: Agent is carcinogenic in experimental animals at a relatively high dose, by route(s) of administration, at site(s), of histologic type(s), or by mechanism(s) not considered relevant to worker exposure. Available epidemologic studies do not confirm an increased risk of cancer in exposed humans. Available evidence suggests that the agent is not likely to cause cancer in humans except under uncommon or unlikely routes or levels of exposure.
EPA-C: Possible human carcinogen: limited evidence of carcinogenicity in animals in the absence of human data.
IARC-3: Not classifiable as to carcinogenicity to humans.
The Registry of Toxic Effects of Chemical Substances (RTECS) contains tumorigenic and/or carcinogenic and/or neoplastic data for this substance.
Reproductive toxicity:
Suspected of damaging fertility or the unborn child.
The Registry of Toxic Effects of Chemical Substances (RTECS) contains reproductive data for this substance.
Specific target organ system toxicity - repeated exposure: No effects known.
Specific target organ system toxicity - single exposure: No effects known.
Aspiration hazard: No effects known.
Subacute to chronic toxicity: The Registry of Toxic Effects of Chemical Substances (RTECS) contains multiple dose toxicity data for this substance.
Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

Toxicity
Aquatic toxicity: No further relevant information available.
Persistence and degradability No further relevant information available.
Bioaccumulative potential No further relevant information available.
Mobility in soil No further relevant information available.
Ecotoxical effects:
Remark: Very toxic for aquatic organisms
Additional ecological information:
General notes:
Do not allow product to reach ground water, water course or sewage system, even in small quantities.
Danger to drinking water if even extremely small quantities leak into the ground.
Also poisonous for fish and plankton in water bodies.
May cause long lasting harmful effects to aquatic life.
Avoid transfer into the environment.
Very toxic for aquatic organisms
Results of PBT and vPvB assessment

PBT:

87-68-3	Hexachloro-1,3-butadiene

vPvB:

87-68-3	Hexachloro-1,3-butadiene

Other adverse effects No further relevant information available.

13 Disposal considerations

Waste treatment methods
Recommendation Consult state, local or national regulations to ensure proper disposal.
Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.

14 Transport information

UN-Number
DOT, IMDG, IATA UN2279

UN proper shipping name
DOT RQ Hexachlorobutadiene
IMDG HEXACHLOROBUTADIENE, MARINE POLLUTANT
IATA HEXACHLOROBUTADIENE

Transport hazard class(es)

DOT

Class 6.1 Toxic substances.
Label 6.1
Class 6.1 (T1) Toxic substances
Label 6.1

IMDG

Class 6.1 Toxic substances.
Label 6.1

IATA

Class 6.1 Toxic substances.
Label 6.1

(Contd. on page 5)

Product name: Hexachloro-1,3-butadiene

(Contd. of page 4)

Packing group **DOT, IMDG, IATA**	III
Environmental hazards: **Marine pollutant (IMDG):**	Environmentally hazardous substance, liquid; Marine Pollutant Yes (PP) Symbol (fish and tree)
Special precautions for user **EMS Number:** **Segregation groups**	Warning: Toxic substances F-A,S-A Liquid halogenated hydrocarbons
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information:	
DOT **Hazardous substance:** **Marine Pollutant (DOT):** **Remarks:**	 1 lbs, 0.454 kg Yes (PP) Special marking with the symbol (fish and tree).
UN "Model Regulation":	UN2279, Hexachlorobutadiene, 6.1, III

15 Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)
Hazard pictograms

GHS06 GHS08

Signal word Danger
Hazard statements
H301 Toxic if swallowed.
H310+H330 Fatal in contact with skin or if inhaled.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H351 Suspected of causing cancer.
H361 Suspected of damaging fertility or the unborn child.
Precautionary statements
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor/…
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P320 Specific treatment is urgent (see on this label).
P361 Take off immediately all contaminated clothing.
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.
National regulations
All components of this product are listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical substance Inventory.
All components of this product are listed on the Canadian Domestic Substances List (DSL).

SARA Section 313 (specific toxic chemical listings)	
87-68-3	Hexachloro-1,3-butadiene

California Proposition 65

Prop 65 - Chemicals known to cause cancer	
87-68-3	Hexachloro-1,3-butadiene

Prop 65 - Developmental toxicity Substance is not listed.
Prop 65 - Developmental toxicity, female Substance is not listed.
Prop 65 - Developmental toxicity, male Substance is not listed.
Information about limitation of use: For use only by technically qualified individuals.
Other regulations, limitations and prohibitive regulations
Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.
The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.
Substance is not listed.
Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.
Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department
Date of preparation / last revision 11/23/2015 / -
Abbreviations and acronyms:
ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
PP: Severe Marine Pollutant
EINECS: European Inventory of Existing Commercial Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
HMIS: Hazardous Materials Identification System (USA)
WHMIS: Workplace Hazardous Materials Information System (Canada)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
vPvB: very Persistent and very Bioaccumulative
ACGIH: American Conference of Governmental Industrial Hygienists (USA)
OSHA: Occupational Safety and Health Administration (USA)
NTP: National Toxicology Program (USA)
IARC: International Agency for Research on Cancer
EPA: Environmental Protection Agency (USA)