

ALFAAA17316

Hexachloro-1,3-butadiene

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明: Product Description:	六氯-1,3-丁二烯 Hexachloro-1,3-butadiene
Cat No. :	A17316
Synonyms	1,1,2,3,4,4-Hexachloro-1,3-butadiene; Perchlorobutadiene; a monomer
CAS No	87-68-3
Molecular Formula	C ₄ Cl ₆
Supplier	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
Emergency Telephone Number	For information US call: 001-800-227-6701 / Europe call: +32 14 57 52 11 Emergency Number US :001-201-796-7100 / Europe : +32 14 57 52 99 CHEMTREC Tel. No. US :001-800-424-9300 / Europe :001-703-527-3887
E-mail address	begel.sdsdesk@thermofisher.com
Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State Liquid	Appearance Yellow	Odor Petroleum distillates
Emergency Overview Toxic if swallowed. Fatal if inhaled. May cause an allergic skin reaction. Suspected of causing genetic defects. Suspected of damaging fertility or the unborn child. Causes damage to organs. Causes damage to organs through prolonged or repeated exposure. Harmful to aquatic life. Very toxic to aquatic life with long lasting effects. Toxic in contact with skin. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation. Suspected of causing cancer.		

Classification of the substance or mixture

Acute Oral Toxicity	Category 3
Acute Dermal Toxicity	Category 3
Acute Inhalation Toxicity - Vapors	Category 1
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Skin Sensitization	Category 1
Germ Cell Mutagenicity	Category 2
Carcinogenicity	Category 2
Reproductive Toxicity	Category 2
Specific target organ toxicity - (single exposure)	Category 1 Category 3
Specific target organ toxicity - (repeated exposure)	Category 1
Acute aquatic toxicity	Category 1 Category 3

Hexachloro-1,3-butadiene

Chronic aquatic toxicity	Category 1
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Label Elements**Signal Word****Danger****Hazard Statements**

H330 - Fatal if inhaled
H317 - May cause an allergic skin reaction
H341 - Suspected of causing genetic defects
H361 - Suspected of damaging fertility or the unborn child
H370 - Causes damage to organs
H372 - Causes damage to organs through prolonged or repeated exposure
H410 - Very toxic to aquatic life with long lasting effects
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation
H351 - Suspected of causing cancer
H301 + H311 - Toxic if swallowed or in contact with skin

Precautionary Statements**Prevention**

P201 - Obtain special instructions before use
P202 - Do not handle until all safety precautions have been read and understood
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P264 - Wash face, hands and any exposed 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
P280 - Wear protective gloves/protective clothing/eye protection/face protection

Response

P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or 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
P311 - Call a POISON CENTER or doctor
P330 - Rinse mouth
P361 + P364 - Take off immediately all contaminated clothing and wash it before reuse
P363 - Wash contaminated clothing before reuse

Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed
P405 - Store locked up

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Physical and Chemical Hazards

None identified.

Health Hazards

Toxic if swallowed. Fatal if inhaled. May cause an allergic skin reaction. Suspected of causing genetic defects. Suspected of damaging fertility or the unborn child. Causes damage to organs. Causes damage to organs through prolonged or repeated exposure. Toxic in contact with skin. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation. Suspected of causing cancer.

Environmental hazards

Harmful to aquatic life. Very toxic to aquatic life with long lasting effects. . Will likely be mobile in the environment due to its water solubility. The product is water soluble, and may spread in water systems.

This product does not contain any known or suspected endocrine disruptors. Toxic to terrestrial vertebrates.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
Hexachlorobutadiene	87-68-3	<=100

SECTION 4. FIRST AID MEASURES

General Advice

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.

Inhalation

Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.

Ingestion

Do NOT induce vomiting. Call a physician or poison control center immediately.

Most important symptoms and effects

None reasonably foreseeable. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

Notes to Physician

Treat symptomatically. Symptoms may be delayed.

SECTION 5. FIRE-FIGHTING MEASURES

Suitable Extinguishing Media

Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Hexachloro-1,3-butadiene

Personal Precautions

Ensure adequate ventilation. Use personal protective equipment as required. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas.

Environmental Precautions

Do not flush into surface water or sanitary sewer system.

Methods for Containment and Clean Up

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE**Handling**

Do not get in eyes, on skin, or on clothing. Wear personal protective equipment/face protection. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance.

Storage

Keep in a dry, cool and well-ventilated place. Keep container tightly closed.

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**Control Parameters**

Component	China	Taiwan	Thailand	Hong Kong
Hexachlorobutadiene	TWA: 0.2 mg/m ³ Skin	TWA: 0.02 ppm TWA: 0.21 mg/m ³		-

Component	ACGIH TLV	OSHA PEL	NIOSH	The United Kingdom	European Union
Hexachlorobutadiene	TWA: 0.02 ppm Skin	(Vacated) TWA: 0.02 ppm (Vacated) TWA: 0.24 mg/m ³	TWA: 0.02 ppm TWA: 0.24 mg/m ³	-	

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

Exposure Controls**Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Viton (R)	See manufacturers recommendations	-	EN 374	(minimum requirement)

Hexachloro-1,3-butadiene

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.
(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure
Respiratory Protection	When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly
Large scale/emergency use	Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387
Small scale/Laboratory use	Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141 When RPE is used a face piece Fit Test should be conducted
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.
Environmental exposure controls	Prevent product from entering drains. Do not allow material to contaminate ground water system. Local authorities should be advised if significant spillages cannot be contained.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	Yellow	
Physical State	Liquid	
Odor	Petroleum distillates	
Odor Threshold	No data available	
pH	Not applicable	
Melting Point/Range	-19 °C / -2.2 °F	
Softening Point	No data available	
Boiling Point/Range	210 - 220 °C / 410 - 428 °F	@ 760 mmHg
Flash Point	No information available	Method - No information available
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Vapor Pressure	29 mbar @ 100 °C	
Vapor Density	8.99 (Air = 1.0)	(Air = 1.0)
Specific Gravity / Density	1.680	
Bulk Density	Not applicable	Liquid
Water Solubility	2.6 g/L (20°C)	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Hexachlorobutadiene	4.9	
Autoignition Temperature	610 °C / 1130 °F	
Decomposition Temperature	No data available	
Viscosity	No data available	
Explosive Properties	No information available	
Oxidizing Properties	No information available	

Molecular Formula C₄ Cl₆
Molecular Weight 260.76

SECTION 10. STABILITY AND REACTIVITY

Stability Stable under normal conditions.

Hazardous Reactions None under normal processing.

Hazardous Polymerization No information available.

Conditions to Avoid Incompatible products.

Materials to avoid Strong oxidizing agents. Strong reducing agents. Metals.

Hazardous Decomposition Products Carbon monoxide (CO). Carbon dioxide (CO₂). Phosgene. Hydrogen chloride gas.

SECTION 11. TOXICOLOGICAL INFORMATION**Product Information****(a) acute toxicity;**

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Hexachlorobutadiene	LD50 = 46 mg/kg (Rat)	LD50 = 1120 mg/kg (Rabbit)	

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory No data available
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; Category 2

The table below indicates whether each agency has listed any ingredient as a carcinogen

Component	EU	UK	Germany	IARC
Hexachlorobutadiene			Cat. 2	

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs Respiratory system

(i) STOT-repeated exposure; No data available

Target Organs None known.

(j) aspiration hazard; No data available

SAFETY DATA SHEET**Hexachloro-1,3-butadiene**

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects Contains a substance which is: Very toxic to aquatic organisms. The product contains following substances which are hazardous for the environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
Hexachlorobutadiene	LC50: 0.2 - 0.3 mg/L, 96h static (Oncorhynchus mykiss) LC50: 0.640 - 0.910 mg/L, 96h static (Lepomis macrochirus) LC50: 0.312 - 0.337 mg/L, 96h flow-through (Lepomis macrochirus) LC50: 0.09 - 0.11 mg/L, 96h flow-through (Pimephales promelas) LC50: 0.268 - 0.381 mg/L, 96h flow-through (Oncorhynchus mykiss)			

Persistence and Degradability**Persistence**

May persist.

Degradation in sewage treatment plant

Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

Bioaccumulative Potential

Product has a high potential to bioconcentrate

Component	log Pow	Bioconcentration factor (BCF)
Hexachlorobutadiene	4.9	No data available

Mobility in soil

The product is water soluble, and may spread in water systems. Will likely be mobile in the environment due to its water solubility. Is not likely mobile in the environment due to its low water solubility and propensity to bind to soil particles.

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

Persistent Organic Pollutant

See table for values

Ozone Depletion Potential

This product does not contain any known or suspected substance

Component	Persistent Organic Pollutant	Ozone Depletion Potential
Hexachlorobutadiene	Annex I - Substance subject to prohibitions Annex III - Substance subject to release reduction Annex IV : 100 mg/kg (Waste Management - Conc. Limit) Annex V : 1000 mg/kg (Waste Management - Max. Conc. Limit) Stockholm Convention - Persistent Organic Pollutant	

SECTION 13. DISPOSAL CONSIDERATIONS**Waste from Residues/Unused Products**

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Hexachloro-1,3-butadiene

Contaminated Packaging Dispose of this container to hazardous or special waste collection point.

Other Information Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport

UN-No UN2279
Proper Shipping Name HEXACHLOROBUTADIENE
Hazard Class 6.1
Packing Group III

IMDG/IMO

UN-No UN2279
Proper Shipping Name HEXACHLOROBUTADIENE
Hazard Class 6.1
Packing Group III

IATA

UN-No UN2279
Proper Shipping Name HEXACHLOROBUTADIENE
Hazard Class 6.1
Packing Group III

Special Precautions for User No special precautions required

SECTION 15. REGULATORY INFORMATION

International Inventories

China, X = listed, Australia, U.S.A. (TSCA), Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Australia (AICS), Korea (KECL), China (IECSC), Japan (ENCS), Philippines (PICCS), Taiwan (TCSI), Japan (ISHL), New Zealand (NZIoC), Japan (ISHL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Hexachlorobutadiene	X	X	X	X	201-765-5	X	X	X	X	X	X	KE-05-0685

National Regulations

Component	Toxic Chemical Substances Control Act
Hexachlorobutadiene 87-68-3 (<=100)	Class I (1 wt%) TRQ = 50 kg

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Revision Date 16-May-2024

Hexachloro-1,3-butadiene

Revision Summary

New emergency telephone response service provider.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Chemical incident response training.

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet