

SAFETY DATA SHEET

Version 6.5
Revision Date 10/26/2021
Print Date 05/28/2022

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : 1,3-Butadiene solution

Product Number : 695904
Brand : Aldrich
CAS-No. : 106-99-0

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

Identified uses : Laboratory chemicals, Synthesis of substances

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

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 2), H225
Skin irritation (Category 2), H315
Germ cell mutagenicity (Category 1B), H340
Reproductive toxicity (Category 2), H361
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336
Specific target organ toxicity - repeated exposure, Inhalation (Category 2), Nervous system, H373
Aspiration hazard (Category 1), H304
Short-term (acute) aquatic hazard (Category 2), H401
Long-term (chronic) aquatic hazard (Category 2), H411

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

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Pictogram



Signal word

Danger

Hazard statement(s)

H225	Highly flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.
H340	May cause genetic defects.
H361	Suspected of damaging fertility or the unborn child.
H373	May cause damage to organs (Nervous system) through prolonged or repeated exposure if inhaled.
H411	Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P260	Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P271	Use only outdoors or in a well-ventilated area.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P331	Do NOT induce vomiting.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391	Collect spillage.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

May form explosive peroxides.

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Formula : C₄H₆
Molecular weight : 54.09 g/mol

Component		Classification	Concentration
n-Hexane			
CAS-No.	110-54-3	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H315, H361, H336, H373, H304, H401, H411 Concentration limits: >= 5 %: STOT RE 2, H373; >= 20 %: STOT SE 3, H336;	>= 70 - < 90 %
EC-No.	203-777-6		
Index-No.	601-037-00-0		
Registration number	01-2119480412-44-XXXX		
1,3-butadiene			
CAS-No.	106-99-0	Flam. Gas 1; Press. Gas Liquefied gas; Muta. 1B; H220, H280, H340	>= 10 - < 20 %
EC-No.	203-450-8		
Index-No.	601-013-00-X		

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

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. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Pay attention to flashback.

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

Forms explosive mixtures with air at ambient temperatures.

5.3 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.

5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 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.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability

Recommended storage temperature
2 - 8 °C

Heat sensitive. Moisture sensitive. Stench. Shock or heat may detonate Handle and store under inert gas.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
n-Hexane	110-54-3	TWA	50 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Danger of cutaneous absorption		
		TWA	50 ppm 180 mg/m ³	USA. NIOSH Recommended Exposure Limits
		TWA	500 ppm 1,800 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	50 ppm 180 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
1,3-butadiene	106-99-0	TWA	2 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Suspected human carcinogen		
		TWA	1 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		STEL	5 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Potential Occupational Carcinogen		

		PEL	1 ppm	OSHA Specifically Regulated Chemicals/Carcinogens
		OSHA specifically regulated carcinogen		
		STEL	5 ppm	OSHA Specifically Regulated Chemicals/Carcinogens
		OSHA specifically regulated carcinogen		
		PEL	1 ppm 2.2 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	5 ppm 11 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
n-Hexane	110-54-3	2,5-Hexanedione	0.5 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift			
1,3-butadiene	106-99-0	1,2-Dihydroxy-4-(N-acetylcysteinyl)-butane	2.5 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			
		Mixture of N-1 and N-2(hydroxybutenyl)valine	2.5 picomoles per gram Hemoglobin	Hemoglobin (Hb) adducts in blood	ACGIH - Biological Exposure Indices (BEI)
		Not critical			

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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). Safety glasses

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: Fluorinated rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min
Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Splash contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Flame retardant antistatic 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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|----------------------------------|
| a) Appearance | Form: liquid
Color: colorless |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | No data available |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point | -76.11 °C (-105.00 °F) |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapor pressure | No data available |
| l) Vapor density | No data available |

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m) Density	0.682 g/cm ³
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	Not classified as explosive.
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

Oxidizing agents, Metals, Copper alloys, Copper, Oxygen, Halogens, Metal oxides, Carbides

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Oral: No data available

Inhalation: No data available

Acute toxicity estimate Dermal - 2,941 mg/kg
(Calculation method)

Skin corrosion/irritation

Mixture causes skin irritation.

Serious eye damage/eye irritation

No data available

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Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Possible mutagen

Carcinogenicity

IARC: 1 - Group 1: Carcinogenic to humans (1,3-butadiene)

NTP: No ingredient 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

Suspected of damaging the unborn child.

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

Mixture may cause damage to organs through prolonged or repeated exposure. - Nervous system

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Components**n-Hexane****Acute toxicity**

LD50 Oral - Rat - male and female - 16,000 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - 4 h - 172 mg/l - vapor

Remarks: (RTECS)

LD50 Dermal - Rabbit - male - > 2,000 mg/kg

(OECD Test Guideline 402)

Remarks: (ECHA)

Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 24 h

(OECD Test Guideline 404)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 72 h
(OECD Test Guideline 405)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative
(OECD Test Guideline 429)

Germ cell mutagenicity

No data available

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Species: Mouse - male

Result: negative

Remarks: (ECHA)

Carcinogenicity

No data available

Reproductive toxicity

Overexposure may cause reproductive disorder(s) based on tests with laboratory animals. Suspected human reproductive toxicant Suspected of damaging fertility. Suspected of damaging fertility.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness. - Central nervous system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure

Inhalation - May cause damage to organs through prolonged or repeated exposure.

- Nervous system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Aspiration hazard

May be fatal if swallowed and enters airways. Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

1,3-butadiene**Acute toxicity**

LD50 Oral - Rat - 5,480 mg/kg

LC50 Inhalation - Rat - 4 h - 285 mg/l - gas

Dermal: No data available

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

In vivo tests showed mutagenic effects

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster lung cells

Result: positive

Method: OECD Test Guideline 474

Species: Mouse - male and female - Bone marrow

Result: positive

Method: OECD Test Guideline 478

Species: Mouse - male

Result: positive

Carcinogenicity

This is or contains a component that has been reported to be carcinogenic based on its IARC, OSHA, ACGIH, NTP, or EPA classification.

Reproductive toxicity

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

SECTION 12: Ecological information**12.1 Toxicity****Mixture**

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Components**n-Hexane**

Toxicity to fish

LC50 - Pimephales promelas (fathead minnow) - 2.5 mg/l - 96 h

Remarks: (ECOTOX Database)

Toxicity to daphnia
and other aquatic
invertebrates

EC50 - Daphnia magna (Water flea) - 2.1 mg/l - 48 h
Remarks: (Lit.)

1,3-butadiene

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 1993 Class: 3 Packing group: II
Proper shipping name: Flammable liquids, n.o.s. (n-Hexane, 1,3-butadiene)
Reportable Quantity (RQ): 66 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 1993 Class: 3 Packing group: II EMS-No: F-E, S-E
Proper shipping name: FLAMMABLE LIQUID, N.O.S. (n-Hexane, 1,3-butadiene)
Marine pollutant : yes

IATA

UN number: 1993 Class: 3 Packing group: II
Proper shipping name: Flammable liquid, n.o.s. (n-Hexane, 1,3-butadiene)

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

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

	CAS-No.	Revision Date
n-Hexane	110-54-3	2020-07-14
1,3-butadiene	106-99-0	2007-07-01

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

SECTION 16: Other information**Further information**

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 applicable to the product with regard to appropriate safety precautions. 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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