

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 8.9

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : (3-Bromo-1-propynyl)benzene solution

Product Number : 728209

Brand : Aldrich

REACH No. : This product is a mixture. REACH Registration Number see section 3.

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

Identified uses : Laboratory chemicals, Manufacture of substances

Uses advised against : For R&D use only. Not for pharmaceutical, household or other uses.

1.3

CHEMIKART

1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Flammable liquids, (Category 2) H225: Highly flammable liquid and vapor.

Acute toxicity, (Category 4) H302: Harmful if swallowed.

Skin irritation, (Category 2) H315: Causes skin irritation.

Serious eye damage, (Category 1) H318: Causes serious eye damage.

Reproductive toxicity, (Category 2)	H361d: Suspected of damaging the unborn child.
Specific target organ toxicity - single exposure, (Category 3), Respiratory system	H336: May cause drowsiness or dizziness.
Specific target organ toxicity - repeated exposure, (Category 2), Central nervous system	H373: May cause damage to organs through prolonged or repeated exposure.
Aspiration hazard, (Category 1)	H304: May be fatal if swallowed and enters airways.
Long-term (chronic) aquatic hazard, (Category 3)	H412: Harmful to aquatic life with long lasting effects.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word	Danger
Hazard Statements	
H225	Highly flammable liquid and vapor.
H302	Harmful if swallowed.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H336	May cause drowsiness or dizziness.
H361d	Suspected of damaging the unborn child.
H373	May cause damage to organs (Central nervous system) through prolonged or repeated exposure.
H412	Harmful to aquatic life with long lasting effects.
Precautionary Statements	
P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
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.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P331	Do NOT induce vomiting.
Supplemental Hazard Statements	none

Reduced Labeling (<= 125 ml)

Pictogram

Signal Word

Danger

Hazard Statements

H304

May be fatal if swallowed and enters airways.

H318

Causes serious eye damage.

H412

Harmful to aquatic life with long lasting effects.

H361d

Suspected of damaging the unborn child.

Precautionary Statements

P280

Wear protective gloves/ protective clothing/ eye protection/ face protection.

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.

P331

Do NOT induce vomiting.

Supplemental Hazard Statements

none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Synonyms : 3-Bromo-1-phenylpropyne solution

Formula : C₉H₇Br

Molecular weight : 195,06 g/mol

Component	Classification	Concentration
(3-Bromo-1-propynyl)benzen		
CAS-No. 1794-48-5	Acute Tox. 4; Eye Dam. 1; H302, H318	>= 70 - < 90 %
*		

Toluene			
CAS-No.	108-88-3	Flam. Liq. 2; Skin Irrit. 2;	>= 30 - < 50 %
EC-No.	203-625-9	Repr. 2; STOT SE 3; STOT	
Index-No.	601-021-00-3	RE 2; Asp. Tox. 1; Aquatic	
Registration	01-2119471310-51-	Chronic 3; H225, H315,	
number	XXXX	H361d, H336, H373, H304, H412 Concentration limits: 20 %: STOT SE 3, H336;	

*A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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. Immediately 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

Water 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

Hydrogen bromide gas

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

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. Suppress (knock down) gases/vapors/mists with a water spray jet. 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.

Storage stability Recommended storage temperature
-20 °C

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

8.2 Exposure controls

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). Tightly fitting safety goggles

Skin protection

required

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.

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.

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) Physical state | clear, liquid |
| b) Color | light green, light yellow |

- | | |
|---|--|
| c) Odor | No data available |
| d) Melting point/freezing point | No data available |
| e) Initial boiling point and boiling range | No data available |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower flammability or explosive limits | No data available |
| h) Flash point | No data available |
| i) Autoignition temperature | No data available |
| j) Decomposition temperature | No data available |
| k) pH | No data available |
| l) Viscosity | Viscosity, kinematic: No data available
Viscosity, dynamic: No data available |
| m) Water solubility | No data available |
| n) Partition coefficient: n-octanol/water | No data available |
| o) Vapor pressure | No data available |
| p) Density | 1,413 g/cm ³ |
| Relative density | No data available |
| q) Relative vapor density | No data available |
| r) Particle characteristics | 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) .
Contains the following stabilizer(s):

Magnesium oxide (0,3 %)

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

Strong oxidizing agents

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

Symptoms: Possible symptoms:, mucosal irritations

Dermal: No data available

Skin corrosion/irritation

Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye damage.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

Reproductive toxicity

Evidence of harm to the unborn child.

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.

- Central nervous system

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

11.2 Additional Information

Endocrine disrupting properties

Product:

Assessment

The substance/mixture does not contain

components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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.

Components

(3-Bromo-1-propynyl)benzen

Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

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

Toluene

Acute toxicity

LD50 Oral - Rat - male - 5.580 mg/kg
(Directive 67/548/EEC, Annex V, B.1.)
LC50 Inhalation - Rat - male - 4 h - 25,7 mg/l - vapor
(OECD Test Guideline 403)
LD50 Dermal - Rabbit - male - > 5.000 mg/kg
Remarks: (ECHA)

Skin corrosion/irritation

Skin - Rabbit
Result: irritating - 4 h
(Regulation (EC) No. 440/2008, Annex, B.4)

Serious eye damage/eye irritation

Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig
Result: negative
(Regulation (EC) No. 440/2008, Annex, B.6)

Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test
Test system: Mouse lymphoma test
Result: negative
Test Type: Ames test
Test system: S. typhimurium
Result: negative
Species: Rat - Bone marrow
Result: negative
Remarks: (ECHA)

Carcinogenicity

No data available

Reproductive toxicity

Suspected of damaging the unborn child.

Specific target organ toxicity - single exposure

Inhalation - 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.
- Central nervous system
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Aspiration hazard

Aspiration may cause pulmonary edema and pneumonitis.

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

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects

No data available

Components

(3-Bromo-1-propynyl)benzen

No data available

Toluene

Toxicity to fish	flow-through test LC50 - Oncorhynchus kisutch (coho salmon) - 5,5 mg/l - 96 h Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Ceriodaphnia dubia (water flea) - 3,78 mg/l - 48 h (US-EPA)
Toxicity to bacteria	static test EC50 - Bacteria - 84 mg/l - 24 h Remarks: (ECHA)
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Oncorhynchus kisutch (coho salmon) - 1,39 mg/l - 40 d Remarks: (ECHA)

Toxicity to daphnia
and other aquatic
invertebrates(Chronic
toxicity)

NOEC - Ceriodaphnia dubia (water flea) - 0,74 mg/l - 7 d
(US-EPA)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1294

IMDG: 1294

IATA: 1294

14.2 UN proper shipping name

ADR/RID: TOLUENE, SOLUTION

IMDG: TOLUENE, SOLUTION

IATA: Toluene, SOLUTION

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA: 3

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA: II

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

14.6 Special precautions for user

Tunnel restriction code : (D/E)

Further information : No data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

Authorisations and/or restrictions on use

REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII) : Toluene

National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

P5c

FLAMMABLE LIQUIDS

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information**Full text of H-Statements**

H225	Highly flammable liquid and vapor.
H302	Harmful if swallowed.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H336	May cause drowsiness or dizziness.
H361d	Suspected of damaging the unborn child.
H373	May cause damage to organs through prolonged or repeated exposure if inhaled.
H412	Harmful to aquatic life with long lasting effects.

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; 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; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; 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 Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; 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; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization 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; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; 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

Classification of the mixture

Flam. Liq.2	H225
Acute Tox.4	H302
Skin Irrit.2	H315
Eye Dam.1	H318
Repr.2	H361d
STOT SE3	H336
STOT RE2	H373
Asp. Tox.1	H304
Aquatic Chronic3	H412

Classification procedure:

Based on product data or assessment
Calculation method
Calculation method
Calculation method
Calculation method
Calculation method
Calculation method
Calculation method

Further information

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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