

• SAFETY DATA SHEET

Version 7.1
Revision Date 11/06/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Phenyllithium solution

Product Number : 593230

Brand : Aldrich

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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 number

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

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Flammable liquids : Category 3

Skin corrosion : Category 1B

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Serious eye damage : Category 1

Specific target organ toxicity - single exposure : Category 3 (Respiratory system)

Short-term (acute) aquatic hazard : Category 3

Long-term (chronic) aquatic hazard : Category 3

Other hazards

Reacts violently with water.

GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H226 Flammable liquid and vapour.
H314 Causes severe skin burns and eye damage.
H335 May cause respiratory irritation.
H412 Harmful to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**
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.
P261 Avoid breathing mist or vapours.
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.

Response:
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.

P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P363 Wash contaminated clothing before reuse.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

Storage:

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.

Disposal:

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

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Mixture
CAS-No. : Not Assigned

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
1,1'-Oxybis(butane)	142-96-1*	>= 70 - < 90	-
phenyllithium	591-51-5*	>= 20 - < 30	-

* Indicates that the identifier is a CAS No.
Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : First aiders need to protect themselves. Show this 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. Call a physician immediately.

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: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.
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
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media : Carbon dioxide (CO₂)
Dry powder

Unsuitable extinguishing media : Water
Foam

Specific hazards during fire fighting : Combustible.

Vapours are heavier than air and may spread along floors.

May not get in touch with: Water

Forms explosive mixtures with air at elevated temperatures.

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

Hazardous combustion products : Carbon oxides

Specific extinguishing : No data available

methods

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

Special protective equipment for fire-fighters : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:
Do not breathe vapours, 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.
Advice for emergency responders:
For personal protection see section 8.

Environmental precautions : Do not let product enter drains.
Risk of explosion.

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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion : Keep away from open flames, hot surfaces and sources of ignition.
Take precautionary measures against static discharge.

Advice on safe handling : Keep workplace dry. Do not allow product to come into contact with water.

Further information on storage conditions : Tightly closed.
Keep away from heat and sources of ignition.

Materials to avoid	: Never allow product to get in contact with water during storage.
Storage class	: 4.2, Pyrophoric and self-heating hazardous materials
Recommended storage temperature	: 36 - 46 °F / 2 - 8 °C
Further information on storage stability	: Handle and store under inert gas. Air and light sensitive.
Packaging material	: Suitable material: Sure-Seal Bottles

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

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.

Hand protection

Material	: Fluorinated rubber
Break through time	: 30 min
Glove thickness	: 0.7 mm
Protective index	: Splash contact
Manufacturer	: Vitoject® (KCL 890 / Aldrich Z677698, Size M)
Manufacturer	: data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

Remarks	: 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. If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE 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.
Eye 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 and body protection	: Flame retardant antistatic protective clothing.
Hygiene measures	: Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: liquid
Color	: No data available
Odor	: No data available
Odor Threshold	: No data available
pH	: No data available
Melting point	: No data available
Boiling point/boiling range	: No data available
Flash point	: 77 °F / 25 °C Method: closed cup
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available

Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: No data available
Relative vapour density	: No data available
Relative density	: No data available
Density	: 0.835 g/cm ³
Water solubility	: No data available
Partition coefficient: n- octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 84.04 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Vapour/air-mixtures are explosive at intense warming.
Chemical stability	: sensitive to moisture
Possibility of hazardous reactions	: No data available

Conditions to avoid : Forms explosive peroxides on prolonged storage
Heating.
Moisture.

Incompatible materials : Strong acids

Hazardous decomposition : In the event of fire: see section 5 products

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Mixture

Acute toxicity

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the oesophagus and the stomach.

Acute toxicity estimate Inhalation - 4 h - 27 mg/l - vapour(Calculation method)

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Dermal: No data available

Skin corrosion/irritation

Remarks: Mixture causes burns.

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye damage.

Risk of blindness!

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component 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

No data available

Specific target organ toxicity - single exposure

Mixture may cause respiratory irritation.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated., Causes severe destruction of the alveolae of the lungs resulting in pulmonary edema, suffocation and possible death. The onset of the pulmonary edema is delayed due to the slow hydrolysis of the material. Long term effects are emphysema, fibrosis, coughing, bloody sputum and general malaise. These symptoms may last several months.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Components

1,1'-Oxybis(butane)

Acute toxicity

LD50 Oral - Rat - male - 7,400 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - male - 4 h - 21.6 mg/l - vapour

(OECD Test Guideline 403)

LD50 Dermal - Rabbit - male - 7,741 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Mild skin irritation - 4 h

(OECD Test Guideline 404)

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

Remarks: Drying-out effect resulting in rough and chapped skin.

Dermatitis

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Moderate eye irritation

(OECD Test Guideline 405)

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

Respiratory or skin sensitization

Open epicutaneous test - Guinea pig

Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test
Test system: Salmonella typhimurium
Result: negative
Test Type: In vitro mammalian cell gene mutation test
Test system: Chinese hamster ovary cells
Result: negative
Test Type: Mutagenicity (mammal cell test): chromosome aberration.
Test system: Human lymphocytes
Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause respiratory irritation.
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

phenyllithium

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: Causes serious eye damage.

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

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

1,1'-Oxybis(butane):

- Toxicity to fish : LC50 (Pimephales promelas (fathead minnow)): 32.3 mg/l
End point: mortality
Exposure time: 96 h
Test Type: flow-through test
Analytical monitoring: yes
Method: OECD Test Guideline 203
- Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): > 18.76 mg/l
End point: Immobilization
Exposure time: 48 h
Test Type: semi-static test
Analytical monitoring: yes
Method: OECD Test Guideline 202
GLP: yes
- Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata (green algae)): ca. 19.1 mg/l
Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 201
GLP: yes
- Toxicity to microorganisms : EC50 (activated sludge): > 1,000 mg/l
Exposure time: 30 min
Test Type: static test
Method: OECD Test Guideline 209
GLP: yes
Remarks: (above the solubility limit in the test medium)

Persistence and degradability

Components:

1,1'-Oxybis(butane):

- Biodegradability : aerobic
Result: Not readily biodegradable.

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Biodegradation: 5 %
Exposure time: 28 d
Method: OECD Test Guideline 301D
GLP: yes

Bioaccumulative potential

Components:

1,1'-Oxybis(butane):

Bioaccumulation : Species: Cyprinus carpio (Carp)
Bioconcentration factor (BCF): 47 - 83
Exposure time: 42 d
Concentration: 0.2 mg/l
Method: OECD Test Guideline 305C

Partition coefficient: n-octanol/water : log Pow: 3.35
Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Components:

1,1'-Oxybis(butane):

Additional ecological information : Avoid release to the environment.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

Not permitted for transport

IMDG-Code

UN number : UN 3392
Proper shipping name : ORGANOMETALLIC SUBSTANCE, LIQUID,
PYROPHORIC
(phenyllithium, 1,1'-Oxybis(butane))
Class : 4.2

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Packing group : I
Labels : 4.2
EmS Code : F-G, S-M
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number : UN 3392
Proper shipping name : Organometallic substance, liquid, pyrophoric
(phenyllithium, 1,1'-Oxybis(butane))
Class : 4.2
Packing group : I
Labels : Division 4.2 - Substances liable to spontaneous
combustion
ERG Code : 135
Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

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

SARA 311/312 Hazards : Fire Hazard
Reactivity Hazard

SARA 313 : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

US State Regulations

Massachusetts Right To Know

1,1'-Oxybis(butane)

142-96-1

Pennsylvania Right To Know

1,1'-Oxybis(butane)

142-96-1

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; 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; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; 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 Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; 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; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation 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; RCRA -

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Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; 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

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