1 Identification

Product identifier

Product name: Phenyllithium, 1.7-1.8M in dibutyl ether

Stock number: 22944
CAS Number:
591-51-5
EC number:
209-720-1
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)


GHS02 Flame

Flam. Liq. 3 H226 Flammable liquid and vapour.
Pyr. Liq. 1 H250 Catches fire spontaneously if exposed to air.
Water-react. 2 H261 In contact with water releases flammable gas.


GHS06 Skull and crossbones

Acute Tox. 3 H301 Toxic if swallowed.
Acute Tox. 3 H311 Toxic in contact with skin.


GHS07

Acute Tox. 4 H332 Harmful if inhaled.
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


GHS02 GHS06

Signal word Danger
Hazard statements
H226 Flammable liquid and vapour.
H250 Catches fire spontaneously if exposed to air.
H261 In contact with water releases flammable gas.
H301+H311 Toxic if swallowed or in contact with skin.
H332 Harmful if inhaled.
Precautionary statements
P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.
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.
P361 Take off immediately all contaminated clothing.
P405 Store locked up.
P422 Store contents under inert gas.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.
WHMIS classification
B2 - Flammable liquid
B6 - Reactive flammable material

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

Health (acute effects) = 3
Flammability = 4
Physical Hazard = 3

Other hazards
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.

(Contd. on page 2)

Product name: Phenyllithium, 1.7-1.8M in dibutyl ether

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3 Composition/information on ingredients

Chemical characterization: Substances
CAS# Description:
591-51-5 Phenyllithium, 1.7-1.8M in dibutyl ether
Identification number(s):
EC number: 209-720-1

4 First-aid measures

Description of first aid measures
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 Seek medical treatment.
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 Extinguishing powder. Do not use water.
For safety reasons unsuitable extinguishing agents Water
Special hazards arising from the substance or mixture
Reacts violently with water
Spontaneously flammable in air.
Substance/product is auto-flammable.
If this product is involved in a fire, the following can be released:
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
Keep away from ignition sources
Environmental precautions: Do not allow material to be released to the environment without proper governmental permits.
Methods and material for containment and cleaning up:
Keep away from ignition sources.
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.
Do not flush with water or aqueous cleansing agents
Prevention of secondary hazards: Keep away from ignition sources.
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
Handle under dry argon.
Keep container tightly sealed.
Store in cool, dry place in tightly closed containers.
Ensure good ventilation at the workplace.
Information about protection against explosions and fires:
Substance/product is self ignitable.
Keep ignition sources away.

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 water/moisture.
Further information about storage conditions:
Protect from humidity and water.
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:

Benzene

		mg/m3	ml/m3
ACGIH	TLV short term	1.6	0.5
ACGIH	TLV long term	8	2.5
B	VME	1,6	0,5
CH	MAK	3,2	1
D	TRGS 900	3,2	1
DK	GV	16	5
F	VME	16	5
GB	MEL	16	5

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I	VME	1,6	0,5
N	TLV	3	1
NL	MAC-TGG	30	10
P	VME	1,6	0,5
S	NGV	1,5	0,5
SF	HTP	16	
USA	PEL short term	3	1 ppm
USA	PEL long term	15	5 ppm

Biphenyl

	ppm
ACGIH TLV	0.2
Australia TWA	0.2
Austria MAK	0.2
Belgium TWA	0.2
Denmark TWA	0.2
Finland TWA	0.2; 0.6-STEL (skin)
France VME	0.2
Germany MAK	0.2
Netherlands MAC-TGG	0.2
Norway TWA	0.2
Poland TWA	0.2; 0.3-STEL
Sweden NGV	0.2; 0.4-STEL
Switzerland MAK-W	0.2
United Kingdom TWA	0.2; 0.6-STEL
OSHA PEL	0.2

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.
Avoid contact with the eyes and skin.
Maintain an ergonomically appropriate working environment.
Breathing equipment: Use suitable respirator when high concentrations are present.
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.
Eye protection:
Safety glasses
Full face protection
Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties	
General Information	
Appearance:	
Form:	Liquid
Odor:	Characteristic
Odor threshold:	Not determined.
pH-value:	Not determined.
Change in condition	
Melting point/Melting range:	Not determined
Boiling point/Boiling range:	Not determined
Sublimation temperature / start:	Not determined
Flash point:	26 °C (79 °F)
Flammability (solid, gaseous)	Not determined.
Ignition temperature:	Not determined
Decomposition temperature:	Not determined
Auto igniting:	Spontaneously flammable in air.
Danger of explosion:	Product is not explosive. However, formation of explosive air/vapor mixtures is possible.
Explosion limits:	
Lower:	Not determined
Upper:	Not determined
Vapor pressure:	Not determined
Density at 20 °C (68 °F):	0.8 g/cm³ (6.676 lbs/gal)
Relative density	Not determined.
Vapor density	Not determined.
Evaporation rate	Not determined.
Solubility in / Miscibility with	
Water:	Reacts violently
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
Reacts violently with water.
Catches fire spontaneously if exposed to air.
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 oxygen
Reacts with alcohols
Reacts with certain metals.

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Product name: Phenyllithium, 1.7-1.8M in dibutyl ether

(Contd. of page 3)

Spontaneously flammable in air.
Reacts violently with water
Conditions to avoid No further relevant information available.
Incompatible materials:
Oxygen
Alcohols
Halogens
Oxidizing agents
Water/moisture
Hazardous decomposition products:
Carbon monoxide and carbon dioxide
Benzene
Metal oxide fume

11 Toxicological information

Information on toxicological effects
Acute toxicity:
Harmful if inhaled.
Toxic in contact with skin.
Toxic if swallowed.
Danger through skin absorption.
LD/LC50 values that are relevant for classification: No data
Skin irritation or corrosion: Irritant to skin and mucous membranes.
Eye irritation or corrosion: Irritating effect.
Sensitization: No sensitizing effects known.
Germ cell mutagenicity: No effects known.
Carcinogenicity:
EPA-A: human carcinogen: sufficient evidence from epidemiologic studies to support a causal association between exposure and cancer.
IARC-1: Carcinogenic to humans: sufficient evidence of carcinogenicity.
ACGIH A1: Confirmed human carcinogen: Agent is carcinogenic to humans based on epidemiologic studies of, or convincing clinical evidence in, exposed humans.
Carcinogen as defined by OSHA.
NTP-K: Known to be carcinogenic: sufficient evidence from human studies.
Reproductive toxicity: No effects known.
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:
Benzene has a strong irritating effect, producing erythema and burning. Edema and blistering is possible in more severe cases. Absorption through the skin may cause the same symptoms as inhalation or ingestion. These include gastrointestinal irritation, low blood pressure, headache, blurred vision, nausea, vomiting, dizziness, loss of balance and coordination, confusion, unconsciousness, coma, respiratory failure and death. Blood, liver and kidney damage is possible. Benzene is a recognized leukemogen and an experimental mutagen and teratogen.
Large amounts of lithium compounds may cause vomiting, diarrhea, ataxia, intestinal irritation, kidney injury, central nervous system depression and a drop in blood pressure. Central nervous system effects may include slurred speech, blurred vision, dizziness, sensory loss, convulsions and stupor. Chronic intake may cause neuromuscular effects such as tremor, ataxia, weakness, clonus and hyperactive reflexes. Lithium can cause kidney damage, gastrointestinal disturbances, fatigue, dehydration, weight loss, dermatological effects and thyroid damage. Lithium ion has shown teratogenic effects in rats and mice.
Dibutyl ether is mildly toxic by inhalation, ingestion and skin contact. Inhalation causes conjunctiva irritation and nasal effects.
Biphenyl is moderately toxic by ingestion and a powerful irritant by inhalation. Human systemic effects include flaccid paralysis, nausea and vomiting. Experimental tumorigen and neoplastigen.
Subacute to chronic toxicity: No effects known.
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.
Additional ecological information:
General notes:
Do not allow material to be released to the environment without proper governmental permits.
Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.
Avoid transfer into the environment.
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.
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**	UN3399
UN proper shipping name **DOT** **IMDG, IATA**	Organometallic substance, liquid, water-reactive, flammable (Phenyllithium) ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE (Phenyllithium)
Transport hazard class(es)	
DOT	
Class	4.3 Substances which, in contact with water, emit flammable gases.
Label	dangerous when wet

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Product name: Phenyllithium, 1.7-1.8M in dibutyl ether

(Contd. of page 4)

Class	4.3 (WF1) Substances which, in contact with water, emit flammable gases
Label	4.3+3
IMDG, IATA	
	
Class	4.3 Substances which, in contact with water, emit flammable gases.
Label	43.+3
Packing group	
DOT, IMDG, IATA	II
Environmental hazards:	Not applicable.
Special precautions for user	Warning: Substances which, in contact with water, emit flammable gases
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information:	
DOT	
Marine Pollutant (DOT):	No
UN "Model Regulation":	UN3399, Organometallic substance, liquid, water-reactive, flammable (Phenyllithium), 4.3 (3), II

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

GHS02 GHS06

Signal word Danger
Hazard statements
H226 Flammable liquid and vapour.
H250 Catches fire spontaneously if exposed to air.
H261 In contact with water releases flammable gas.
H301+H311 Toxic if swallowed or in contact with skin.
H332 Harmful if inhaled.
Precautionary statements
P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.
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.
P361 Take off immediately all contaminated clothing.
P405 Store locked up.
P422 Store contents under inert gas.
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.
The components of this product are listed on the Canadian Domestic Substances List (DSL) and/or the Canadian Non-Domestic Substances List (NDSL).
SARA Section 313 (specific toxic chemical listings) Substance is not listed.
California Proposition 65
Prop 65 - Chemicals known to cause cancer Substance is not listed.
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.
This product contains benzene and is subject to the reporting requirements of section 313 of the Emergency Planning and Community Right to Know Act of 1986 and 40CFR372.
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:
RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)
IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)
ICAO: International Civil Aviation Organization
ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)
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
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)