

SAFETY DATA SHEET

Creation Date 24-Nov-2010

Revision Date 06-Jan-2023

Revision Number 8

1. Identification

Product Name tert-Butyllithium, 1.9M solution in pentane

Cat No. : AC396540000; AC396541000; AC396548000

Synonyms No information available

Recommended Use Laboratory chemicals.

Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number

For information **US** call: 001-800-ACROS-01 / **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

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 1
Substances/mixtures which, in contact with water, emit flammable gases	Category 1
Pyrophoric liquids	Category 1
Skin Corrosion/Irritation	Category 1 B
Serious Eye Damage/Eye Irritation	Category 1
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system, Central nervous system (CNS).	
Aspiration Toxicity	Category 1

Label Elements

Signal Word

Danger

Hazard Statements

Extremely flammable liquid and vapor
In contact with water releases flammable gases which may ignite spontaneously
Catches fire spontaneously if exposed to air
May be fatal if swallowed and enters airways
Causes severe skin burns and eye damage
May cause respiratory irritation
May cause drowsiness or dizziness



Precautionary Statements

Prevention

Do not breathe dust/fume/gas/mist/vapors/spray
Wash face, hands and any exposed skin thoroughly after handling
Wear protective gloves/protective clothing/eye protection/face protection
Use only outdoors or in a well-ventilated area
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep container tightly closed
Ground/bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting equipment
Use only non-sparking tools
Take precautionary measures against static discharge
Do not allow contact with air
Keep away from any possible contact with water, because of violent reaction and possible flash fire
Handle under inert gas. Protect from moisture
Keep cool

Response

Immediately call a POISON CENTER or doctor/physician

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

Skin

Wash contaminated clothing before reuse
IF ON SKIN: Immerse in cool water/wrap with wet bandages
Brush off loose particles from skin. Immerse in cool water/wrap with wet bandages

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

Ingestion

Do NOT induce vomiting
Rinse mouth

Fire

In case of fire: Use limestone powder, sodium chloride or dry sand to extinguish

Storage

Store locked up
Store in a well-ventilated place. Keep container tightly closed
Store contents under inert gas
Store in a dry place. Store in a closed container

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

Toxic to aquatic life with long lasting effects
Reacts violently with water

3. Composition/Information on Ingredients

Component	CAS No	Weight %
Pentane	109-66-0	50-65
Lithium, (1,1-dimethylethyl)-	594-19-4	10-25
Isopentane	78-78-4	20-25

4. First-aid measures

General Advice	Immediate medical attention is required. Show this safety data sheet to the doctor in attendance.
Eye Contact	Immediate medical attention is required. Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Keep eye wide open while rinsing.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Call a physician immediately.
Inhalation	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. Remove from exposure, lie down. Risk of serious damage to the lungs (by aspiration). Call a physician immediately.
Ingestion	Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Call a physician immediately. Clean mouth with water. Call a physician or poison control center immediately. If vomiting occurs naturally, have victim lean forward.
Most important symptoms and effects	Causes burns by all exposure routes. Difficulty in breathing. . Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation: Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Dry sodium chloride. Limestone powder. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	Water, Carbon dioxide (CO2), Foam
Flash Point	-56 °C / -68.8 °F
Method -	Pentane
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Extremely flammable. Reacts violently with water. The product causes burns of eyes, skin and mucous membranes. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

Hazardous Combustion Products

Carbon oxides. Carbon monoxide (CO). Carbon dioxide (CO₂). Isobutane.

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.

NFPA

Health
3

Flammability
4

Instability
3

Physical hazards
W

6. Accidental release measures**Personal Precautions**

Use personal protective equipment as required. Ensure adequate ventilation. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak. Remove all sources of ignition. Take precautionary measures against static discharges.

Environmental Precautions

Do not flush into surface water or sanitary sewer system. See Section 12 for additional Ecological Information. Avoid release to the environment. Collect spillage.

Methods for Containment and Clean Up

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Do not expose spill to water. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

7. Handling and storage**Handling**

Use only under a chemical fume hood. Handle under inert gas, protect from moisture. Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Do not allow contact with water. Keep away from open flames, hot surfaces and sources of ignition. Use spark-proof tools and explosion-proof equipment. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.

Storage.

Keep containers tightly closed in a dry, cool and well-ventilated place. Corrosives area. Keep away from water or moist air. Keep away from heat, sparks and flame. Flammables area. To maintain product quality: Keep refrigerated. Incompatible Materials. Acids. Alcohols. Keep from any possible contact with water, because of violent reaction and possible flash fire.

8. Exposure controls / personal protection**Exposure Guidelines**

Component	ACGIH TLV	OSHA PEL	NIOSH	Mexico OEL (TWA)
Pentane	TWA: 1000 ppm	(Vacated) TWA: 600 ppm (Vacated) TWA: 1800 mg/m ³ (Vacated) STEL: 750 ppm (Vacated) STEL: 2250 mg/m ³ TWA: 1000 ppm TWA: 2950 mg/m ³	IDLH: 1500 ppm TWA: 120 ppm TWA: 350 mg/m ³ Ceiling: 610 ppm Ceiling: 1800 mg/m ³	TWA: 600 ppm
Isopentane	TWA: 1000 ppm			TWA: 600 ppm

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

Engineering Measures

Use only under a chemical fume hood. Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation

location. Ensure adequate ventilation, especially in confined areas.

Personal Protective Equipment

Eye/face Protection	Tight sealing safety goggles. Face protection shield.
Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure.
Respiratory Protection	Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Recommended Filter type:	low boiling organic solvent. Type AX. Brown. conforming to EN371. or. Organic gases and vapours filter. Type A. Brown. conforming to EN14387.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Yellow
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	No data available
Boiling Point/Range	No information available
Flash Point	-56 °C / -68.8 °F
Method -	Pentane
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	No information available
Specific Gravity	0.690
Solubility	Reacts violently with water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C ₄ H ₉ Li
Molecular Weight	64.04

10. Stability and reactivity

Reactive Hazard	Yes
Stability	Pyrophoric: Spontaneously flammable in air. Water reactive.
Conditions to Avoid	Incompatible products. Excess heat. Exposure to moist air or water. Exposure to moisture. Keep away from open flames, hot surfaces and sources of ignition.
Incompatible Materials	Acids, Alcohols, Keep from any possible contact with water, because of violent reaction and possible flash fire
Hazardous Decomposition Products	Carbon oxides, Carbon monoxide (CO), Carbon dioxide (CO ₂), Isobutane
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	Reacts violently with water. Pyrophoric: Spontaneously flammable in air.

11. Toxicological information

Acute Toxicity

Product Information

No acute toxicity information is available for this product

Oral LD50

Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.

Dermal LD50

Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.

Vapor LC50

Based on ATE data, the classification criteria are not met. ATE > 20 mg/l.

Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Pentane	LD50 > 2000 mg/kg (Rat)	LD50 = 3000 mg/kg (Rabbit)	LC50 = 364 g/m ³ (Rat) 4 h

Toxicologically Synergistic Products

No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation

Causes burns by all exposure routes

Sensitization

No information available

Carcinogenicity

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

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Pentane	109-66-0	Not listed	Not listed	Not listed	Not listed	Not listed
Lithium, (1,1-dimethylethyl)-	594-19-4	Not listed	Not listed	Not listed	Not listed	Not listed
Isopentane	78-78-4	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects

No information available

Reproductive Effects

No information available.

Developmental Effects

No information available.

Teratogenicity

No information available.

STOT - single exposure

Respiratory system Central nervous system (CNS)

STOT - repeated exposure

None known

Aspiration hazard

No information available

Symptoms / effects, both acute and delayed

Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation: Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

Endocrine Disruptor Information

No information available

Other Adverse Effects

The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information.

12. Ecological information

Ecotoxicity

Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment. Reacts with water so no ecotoxicity data for the substance is available.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Pentane	Not listed	LC50: = 9.99 mg/L, 96h (Lepomis macrochirus)	Not listed	EC50: = 9.74 mg/L, 48h (Daphnia magna)

		LC50: = 11.59 mg/L, 96h (Pimephales promelas) LC50: = 9.87 mg/L, 96h (Oncorhynchus mykiss)		
Isopentane	Not listed	Oncorhynchus mykiss: LC50: 3.1 mg/L/96h	Not listed	EC50: = 2.3 mg/L, 48h (Daphnia magna)

Persistence and Degradability Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility . Is not likely mobile in the environment.

Component	log Pow
Pentane	3.45
Isopentane	4

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

UN-No UN3394
 Proper Shipping Name ORGANOMETALLIC SUBSTANCE, LIQUID, PYROPHORIC, WATER-REACTIVE
 Technical Name (TERT-BUTYLLITHIUM, PENTANE)
 Hazard Class 4.2
 Subsidiary Hazard Class 4.3, 3, 8
 Packing Group I

TDG

UN-No UN3394
 Proper Shipping Name ORGANOMETALLIC SUBSTANCE, LIQUID, PYROPHORIC, WATER-REACTIVE
 Hazard Class 4.2
 Subsidiary Hazard Class 4.3, 3, 8
 Packing Group I

IATA

UN-No UN3394
 Proper Shipping Name ORGANOMETALLIC SUBSTANCE, LIQUID, PYROPHORIC, WATER-REACTIVE,
 FORBIDDEN FOR IATA TRANSPORT
 Hazard Class 4.2
 Subsidiary Hazard Class 4.3
 Packing Group I

IMDG/IMO

UN-No UN3394
 Proper Shipping Name ORGANOMETALLIC SUBSTANCE, LIQUID, PYROPHORIC, WATER-REACTIVE
 Hazard Class 4.2
 Subsidiary Hazard Class 4.3
 Packing Group I

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Pentane	109-66-0	X	ACTIVE	-
Lithium, (1,1-dimethylethyl)-	594-19-4	X	ACTIVE	-
Isopentane	78-78-4	X	ACTIVE	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

- - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)

Not applicable

TSCA 12(b) - Notices of Export

Not applicable

International Inventories

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Pentane	109-66-0	X	-	203-692-4	X	X	X	X	X	KE-27968
Lithium, (1,1-dimethylethyl)-	594-19-4	-	X	209-831-5	X	X	X	X	X	2014-3-6117
Isopentane	78-78-4	X	-	201-142-8	X	X	X	X	X	KE-23537

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)**U.S. Federal Regulations****SARA 313**

Not applicable

SARA 311/312 Hazard Categories

See section 2 for more information

CWA (Clean Water Act)

Not applicable

Clean Air Act

Not applicable

OSHA - Occupational Safety and Health Administration

Not applicable

CERCLA

Not applicable

California Proposition 65

This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Pentane	X	X	X	-	X
Isopentane	X	X	X	-	-

U.S. Department of Transportation

Reportable Quantity (RQ): N

DOT Marine Pollutant N

DOT Severe Marine Pollutant N

U.S. Department of Homeland Security

This product contains the following DHS chemicals:

Legend - STQs = Screening Threshold Quantities, APA = A placarded amount

Component	DHS Chemical Facility Anti-Terrorism Standard
Pentane	Release STQs - 10000lb
Isopentane	Release STQs - 10000lb

Other International Regulations**Mexico - Grade**

No information available

Authorisation/Restrictions according to EU REACH

Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Pentane	109-66-0	-	-	-
Lithium, (1,1-dimethylethyl)-	594-19-4	-	-	-
Isopentane	78-78-4	-	-	-

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Pentane	109-66-0	Listed	Not applicable	Not applicable	Not applicable
Lithium, (1,1-dimethylethyl)-	594-19-4	Not applicable	Not applicable	Not applicable	Not applicable
Isopentane	78-78-4	Listed	Not applicable	Not applicable	Not applicable

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Pentane	109-66-0	Not applicable	Not applicable	Not applicable	Not applicable
Lithium, (1,1-dimethylethyl)-	594-19-4	Not applicable	Not applicable	Not applicable	Not applicable
Isopentane	78-78-4	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By

Regulatory Affairs
Thermo Fisher Scientific
Email: EMSDS.RA@thermofisher.com

Creation Date

24-Nov-2010

Revision Date

06-Jan-2023

Print Date

06-Jan-2023

Revision Summary

This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

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 SDS