# Material Safety Data Sheet
## n-Butyllithium, 2.5M solution in hexanes

ACC# 66360

## Section 1 - Chemical Product and Company Identification

**MSDS Name:** n-Butyllithium, 2.5M solution in hexanes
**Catalog Numbers:** AC213350000, AC213350150, AC213351000, AC213351300, AC213358000
**Synonyms:** None.
**Company Identification:**

Acros Organics N.V.
One Reagent Lane
Fair Lawn, NJ 07410

**For information in North America, call:** 800-ACROS-01
**For emergencies in the US, call CHEMTREC:** 800-424-9300

## Section 2 - Composition, Information on Ingredients

| CAS# | Chemical Name | Percent | EINECS/ELINCS |
|---|---|---|---|
| 110-54-3 | Hexane | 85-88 | 203-777-6 |
| 109-72-8 | n-Butyllithium | 12-15 | 203-698-7 |

## Section 3 - Hazards Identification

### EMERGENCY OVERVIEW

Appearance: clear yellow solid/liquid mixture. Flash Point: -21 deg C.
**Danger! Extremely flammable liquid.** Water-reactive. Corrosive. Causes severe eye and skin burns. Causes digestive and respiratory tract burns. Pyrophoric. Spontaneously flammable in air. Aspiration hazard if swallowed. Can enter lungs and cause damage. May cause central nervous system depression. May cause kidney damage. Hygroscopic (absorbs moisture from the air).
**Target Organs:** Kidneys, central nervous system.

### Potential Health Effects

**Eye:** Causes severe eye burns. May cause irreversible eye injury.
**Skin:** Contact with liquid is corrosive and causes severe burns and ulceration.
**Ingestion:** Aspiration hazard. May cause central nervous system depression, kidney damage, and liver damage. Causes digestive tract burns with immediate pain, swelling of the throat, convulsions, and possible coma. Aspiration of material into the lungs may cause chemical pneumonitis, which may be fatal. May cause corrosion and permanent tissue destruction of the esophagus and digestive tract. May cause ear ringing, blurred vision, thyroid abnormalities, photophobia, coma, and seizures. The characteristics of lithium toxicity include: tremors, nausea, slurred speech, sluggishness, vertigo, thirst, and increased urine output. Effects from continued exposure include apathy, anorexia, fatigue, lethargy, muscular weakness, and cardiac changes. Long term exposure may lead to hypothroidism, leukocytosis, edema, weight gain, memory impairment, seizures, kidney damage, shock, hypotennsion, cardiac arrhythmias, coma, and death. Lithium has been implicated in the development of aplastic anemia.
**Inhalation:** Inhalation of high concentrations may cause central nervous system effects characterized by nausea, headache, dizziness, unconsciousness and coma. Irritation may lead to chemical pneumonitis and pulmonary edema. Causes severe irritation of upper respiratory tract with coughing, burns, breathing difficulty, and possible coma. May cause effects similar to those described for ingestion.
**Chronic:** Chronic inhalation and ingestion may cause effects similar to those of acute inhalation and ingestion. Chronic exposure may cause kidney damage.

## Section 4 - First Aid Measures

**Eyes:** Get medical aid immediately. Do NOT allow victim to rub eyes or keep eyes closed. Extensive irrigation with water is required (at least 30 minutes).
**Skin:** Get medical aid immediately. Flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Destroy contaminated shoes.
**Ingestion:** Do not induce vomiting. If victim is conscious and alert, give 2-4 cupfuls of milk or water. Possible aspiration hazard. Get medical aid immediately.
**Inhalation:** Get medical aid immediately. Remove from exposure and move to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Do NOT use mouth-to-mouth resuscitation. If breathing has ceased apply artificial respiration using oxygen and a suitable mechanical device such as a bag and a mask.
**Notes to Physician:** Treat symptomatically and supportively.

## Section 5 - Fire Fighting Measures

**General Information:** Evacuate area and fight fire from a safe distance. Containers can build up pressure if exposed to heat and/or fire. As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Vapors can travel to a source of ignition and flash back. Combustion generates toxic fumes. Material is easily ignited if allowed to dry. Extremely flammable. Material will readily ignite at room temperature. Water Reactive. Material will react with water and may release a flammable and/or toxic gas. Use water spray to keep fire-exposed containers cool. Water may be ineffective. Material is lighter than water and a fire may be spread by the use of water. Can form explosive mixtures at temperatures above the flashpoint. Vapors may be heavier than air. They can spread along the ground and collect in low or confined areas.
**Extinguishing Media:** Water may be ineffective. Do NOT use carbon dioxide. DO NOT USE WATER! Use dry chemical. Do NOT use

straight streams of water. Cool containers with flooding quantities of water until well after fire is out.
**Flash Point:** -21 deg C ( -5.80 deg F)
**Autoignition Temperature:** 240 deg C ( 464.00 deg F)
**Explosion Limits, Lower:**1.20 vol %
**Upper:** 7.40 vol %
**NFPA Rating:** (estimated) Health: 3; Flammability: 4; Instability: 2; Special Hazard: -W-

## Section 6 - Accidental Release Measures

**General Information:** Use proper personal protective equipment as indicated in Section 8.
**Spills/Leaks:** Avoid runoff into storm sewers and ditches which lead to waterways. Clean up spills immediately, observing precautions in the Protective Equipment section. Scoop up with a nonsparking tool, then place into a suitable container for disposal. Remove all sources of ignition. Absorb spill using an absorbent, non-combustible material such as earth, sand, or vermiculite. Do not use combustible materials such as sawdust. Provide ventilation.

## Section 7 - Handling and Storage

**Handling:** Remove contaminated clothing and wash before reuse. Ground and bond containers when transferring material. Do not get in eyes, on skin, or on clothing. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep container tightly closed. Do not ingest or inhale. Do not allow contact with water. Use only in a chemical fume hood. Store and handle protected from air. Do not use if the material has evaporated to dryness. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames.
**Storage:** Keep away from heat, sparks, and flame. Keep away from sources of ignition. Keep container closed to prevent drying out. Keep under a nitrogen blanket. Keep from contact with oxidizing materials. Store in a cool, dry, well-ventilated area away from incompatible substances. Keep away from water. Keep away from organic halogens. Refrigerator/flammables.

## Section 8 - Exposure Controls, Personal Protection

**Engineering Controls:** Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Use adequate general or local explosion-proof ventilation to keep airborne levels to acceptable levels.
**Exposure Limits**

| Chemical Name | ACGIH | NIOSH | OSHA - Final PELs |
|---|---|---|---|
| Hexane | 50 ppm TWA; Skin - potential significant contribution to overall exposure by the cutaneous r oute | 50 ppm TWA; 180 mg/m3 TWA 1100 ppm IDLH | 500 ppm TWA; 1800 mg/m3 TWA |
| n-Butyllithium | none listed | none listed | none listed |

**OSHA Vacated PELs:** Hexane: 50 ppm TWA; 180 mg/m3 TWA n-Butyllithium: No OSHA Vacated PELs are listed for this chemical.
**Personal Protective Equipment**
**Eyes:** Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
**Skin:** Wear appropriate protective gloves to prevent skin exposure.
**Clothing:** Wear appropriate protective clothing to minimize contact with skin.
**Respirators:** 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.

## Section 9 - Physical and Chemical Properties

**Physical State:** Solid/Liquid Mixture
**Appearance:** clear yellow
**Odor:** hexane-like
**pH:** Not available.
**Vapor Pressure:** 160 mbar @ 20 deg C
**Vapor Density:** Not available.
**Evaporation Rate:**Not available.
**Viscosity:** 0.38mPas 20 deg C
**Boiling Point:** 60 - 80 deg C @ 760.00mm Hg
**Freezing/Melting Point:**-95 deg C
**Decomposition Temperature:**Not available.
**Solubility:** reacts
**Specific Gravity/Density:**.6800g/cm3
**Molecular Formula:**C4H9Li
**Molecular Weight:**64.06

## Section 10 - Stability and Reactivity

**Chemical Stability:** Stable under normal temperatures and pressures.
**Conditions to Avoid:** Incompatible materials, ignition sources, exposure to air, contact with water, organic materials, strong oxidants, exposure to moist air or water, dehydrating agents.
**Incompatibilities with Other Materials:** Lithium is incompatible with acetonitrile + sulfur dioxide, bromine pentafluoride, bromobenzene, carbon + lithium tetrachloroaluminate + sulfunyl chloride, carbon + sulfunyl chloride, chlorine tri or pentafluoride, diazomethane, diborane, ethylene, halocarbbons, halogens, hydrogen, mercury, metal chlorides + nitrogen, metal oxides and chalcogenides, metals, nitric acid, nitryly fluoride, non-metal oxides, platinum, pol(1,1-difluoroethylene-hexafluoropropylene) (viton), sodium carbonate, sulfur, sulfinyl chloride, sulfur dioxide, trifluoromethyl hypofluorite, halocarbons, halogens, iron(II) sulfide, manganese telluride, arsenic, beryllium, maleic

anhydride, carbides, carbon dioxide, + water, chlorine, chromium, chromium trichloride, cobalt alloys, nickel alloys, nitrogen, organic matter, oxygen, phosphorus, rubber, silicates, sodium nitrite, tantalum (V) oxide, vanadium, zirconium tetrachloride, iodoform, nitrogen + metal chlorides, fluorine, magnesium perchlorate. Butyl lithium above 20% in air can ignite spontaneously if the humidity exceeds 70%. Concentrations above 25% are pyrophoric at any humidity. Hexane is incompatible with dinitrogen tetraoxide.
**Hazardous Decomposition Products:** Carbon monoxide, irritating and toxic fumes and gases, carbon dioxide, lithium hydroxide, butane, oxides of lithium.
**Hazardous Polymerization:** Has not been reported.

## Section 11 - Toxicological Information

**RTECS#:**
**CAS#** 110-54-3: MN9275000
**CAS#** 109-72-8 unlisted.
**LD50/LC50:**
CAS# 110-54-3:
Draize test, rabbit, eye: 10 mg Mild;
Inhalation, mouse: LC50 = 150000 mg/m3/2H;
Inhalation, rat: LC50 = 48000 ppm/4H;
Inhalation, rat: LC50 = 627000 mg/m3/3M;
Oral, rat: LD50 = 25 gm/kg;
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CAS# 109-72-8:
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**Carcinogenicity:**
CAS# 110-54-3: Not listed by ACGIH, IARC, NTP, or CA Prop 65.
CAS# 109-72-8: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

**Epidemiology:** No information available.
**Teratogenicity:** No information available.
**Reproductive Effects:** No information available.
**Mutagenicity:** No information available.
**Neurotoxicity:** No information available.
**Other Studies:**

## Section 12 - Ecological Information

**Ecotoxicity:** No data available. Cas# 110-54-3:LC50(96Hr.) Rainbow Trout = 4.14 mg/L; Flow-through BioassayLC50(96Hr.)Fathead Minnow=5.10 mg/LLC50(96Hr.)Bluegill = 4.12 mg/LLC50 (48Hr.) Water Flea = 3.87 mg/L
**Environmental:** Hexane is expected to rapidly volatilize leaving a deposit of N-Butyllithium behind. Based upon a water solubility of 9.5 mg/l at 25 deg C and a log Kow of 4.11, the bioconcentration factor (log BCF) for n-hexane has been calculated to be 2.24 and 2.89, respectively, from recommended regression derived equations. These bioconcentration factor values are not indicative of important bioconcentration in aquatic organisms.
**Physical:** Photolysis or hydrolysis of n-hexane in aquatic systems are not expected to be important. The log biodegradation of n-hexane may occur in aquatic environments; however, volatilization and adsorption are expected to be far more important fate processes.
**Other:** o not empty into drains.

## Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.
**RCRA P-Series:** None listed.
**RCRA U-Series:** None listed.

## Section 14 - Transport Information

| | US DOT | Canada TDG |
|---|---|---|
| **Shipping Name:** | ORGANOMETALLIC SUBSTANCE, LIQUID, PYROPHORIC, WATER-REACTIVE | LITHIUM ALKYLS |
| **Hazard Class:** | 4.2 | 4.2(4.3) |
| **UN Number:** | UN3394 | UN2445 |
| **Packing Group:** | I | I |

## Section 15 - Regulatory Information

### US FEDERAL

**TSCA**
CAS# 110-54-3 is listed on the TSCA inventory.
CAS# 109-72-8 is listed on the TSCA inventory.
**Health & Safety Reporting List**
None of the chemicals are on the Health & Safety Reporting List.
**Chemical Test Rules**

None of the chemicals in this product are under a Chemical Test Rule.

**Section 12b**

None of the chemicals are listed under TSCA Section 12b.

**TSCA Significant New Use Rule**

None of the chemicals in this material have a SNUR under TSCA.

**CERCLA Hazardous Substances and corresponding RQs**

CAS# 110-54-3: 5000 lb final RQ; 2270 kg final RQ

**SARA Section 302 Extremely Hazardous Substances**

None of the chemicals in this product have a TPQ.

**SARA Codes**

CAS # 110-54-3: immediate, delayed, fire.

**Section 313**

This material contains Hexane (CAS# 110-54-3, 85-88%),which is subject to the reporting requirements of Section 313 of SARA Title III and 40 CFR Part 373.

**Clean Air Act:**

CAS# 110-54-3 is listed as a hazardous air pollutant (HAP).

This material does not contain any Class 1 Ozone depletors.
This material does not contain any Class 2 Ozone depletors.

**Clean Water Act:**

None of the chemicals in this product are listed as Hazardous Substances under the CWA.
None of the chemicals in this product are listed as Priority Pollutants under the CWA.
None of the chemicals in this product are listed as Toxic Pollutants under the CWA.

**OSHA:**

None of the chemicals in this product are considered highly hazardous by OSHA.

**STATE**

CAS# 110-54-3 can be found on the following state right to know lists: New Jersey, Pennsylvania, Minnesota, Massachusetts.
CAS# 109-72-8 can be found on the following state right to know lists: New Jersey, Pennsylvania.

**California Prop 65**

California No Significant Risk Level: None of the chemicals in this product are listed.

## European/International Regulations

**European Labeling in Accordance with EC Directives**

**Hazard Symbols:**

F C

**Risk Phrases:**

R 11 Highly flammable.
R 14/15 Reacts violently with water liberating extremely flammable gases.
R 17 Spontaneously flammable in air.
R 34 Causes burns.
R 48/20 Harmful : danger of serious damage to health by prolonged exposure through inhalation.
R 62 Possible risk of impaired fertility.
R 51/53 Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
R 65 Harmful: may cause lung damage if swallowed.
R 67 Vapours may cause drowsiness and dizziness.

**Safety Phrases:**

S 16 Keep away from sources of ignition - No smoking.
S 33 Take precautionary measures against static discharges.
S 6A Keep under nitrogen.
S 43B In case of fire, use fire-fighting equipment on basis of sodium chloride, sodium bicarbonate (never use water).

**WGK (Water Danger/Protection)**

CAS# 110-54-3: 1
CAS# 109-72-8: 2

**Canada - DSL/NDSL**

CAS# 110-54-3 is listed on Canada's DSL List.
CAS# 109-72-8 is listed on Canada's DSL List.

**Canada - WHMIS**

This product has a WHMIS classification of B2, E, B6.
This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

**Canadian Ingredient Disclosure List**

CAS# 110-54-3 is listed on the Canadian Ingredient Disclosure List.

## Section 16 - Additional Information

**MSDS Creation Date:** 6/03/1999
**Revision #5 Date:** 10/05/2004