



SAFETY DATA SHEET LITHIUM TRI-TERT-BUTOXYALUMINUM HYDRIDE IN THF

1. Identification of the Substance/Mixture and of the Company/Undertaking:

- 1.1 **Product Identifier:** Lithium tri-tert-butoxyaluminum hydride in tetrahydrofuran
- 1.1.1 **Substances** Not applicable
- 1.1.2 **Mixture name:** Lithium tri-tert-butoxyaluminum hydride in tetrahydrofuran
- Alternate names and trade name** TBLAH in THF
- 1.2 **Relevant Identified Uses of the Substance or Mixture and Uses Advised Against:**
Industrial Manufacturing
Only to be supplied for industrial uses
For use only as a chemical intermediate under Strictly Controlled Conditions.

1.3 **Details of the Supplier of the Safety Data Sheet**

North America
FMC Corporation
2801 Yorkmont Road, Suite 300
Charlotte, NC 28208
Phone: +1.704.426.5300
Fax: +1.704.426.5370
1.888.lithium

Europe
FMC Chemicals
Commercial Road
Bromborough, Merseyside
CH62 3NL, England
Phone: +44.151. 334.8085
Fax: +44.151.482.7361

Asia Pacific
FMC Asia Innovation Center
No 3 Building No. 4560
Jinke Road
Shanghai, China 201203
T: +86.21.2067.5888

Email: lithium.info@fmc.com
Web: www.fmclithium.com

1.4 **Emergency Telephone Number:**

North America
CHEMTREC: +1.800.424.9300
+1.703.527.3887
Plant: +1.704.629.5361
Medical: +1.303.595.9048

Europe
24 hr Specialist advice number:
CHEMTREC: +44 870 8200418

Asia Pacific
Phone: +86.21.2067.5888

2. Hazards Identification

2.1 **Classification of the Mixture:**

2.1.1 GHS Classification [EC Regulation No 1272/2008 and US OSHA regulations]

Water reactive; Category 1
Flammable liquid; Category 2
Skin corrosive; Category 1B
Eye damage; Category 1
Carcinogen; Category 2
Specific target organ systemic toxicity – SE Category 3
Acute Toxicity; Category 4 (inhalation)

2.2.2 EC: Classification according to 67/548/EEC or 1999/45/EC [DSD/DPD]

F; R11, R14/15, C; R34, Carc. Cat.3; R40, Xi; R37, Xn; R20

2.2 Label Elements:
2.2.3 Hazard Pictograms:



2.2.4 Signal Word:
Hazard Statement(s):

Danger	
In contact with water releases flammable gases, which may ignite spontaneously.	H260
Highly flammable liquid and vapour.	H225
Causes severe skin burns and eye damage.	H314
Harmful if inhaled.	H332
Suspected of causing cancer.	H351
May cause respiratory irritation.	H335

Precautionary Statement(s):

Handle under inert gas. Protect from moisture.	P231 + P232
In case of fire: Use dry chemical for extinction.	P370 + P378
Wear protective gloves/protective clothing/eye protection/ face protection.	P280
IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.	P301 + P330 + P331
IF ON SKIN (or hair): Remove / Take off immediately all contaminated clothing. Rinse skin with water / shower.	P303 + P361 + P353
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.	P305 + P351 + P338
Immediately call a POISON Center or doctor/physician.	P310

Additional Precautionary Statement(s):

Obtain special instructions before use.	P201
Do not handle until all safety precautions have been read and understood.	P202
Keep away from heat/sparks/open flames/hot surfaces. – No smoking.	P210
Keep away from any possible contact with water, because of violent reaction and possible flash fire.	P223
Ground/bond container and receiving equipment.	P240
Use explosion-proof electrical, ventilating and lighting equipment.	P241
Use only non-sparking tools.	P242
Take precautionary measures against static discharge.	P243
Do not breathe gas, fume, vapours or spray.	P260
Wash hands thoroughly after handling.	P264
Use only outdoors or in a well-ventilated area.	P271
Use personal protective equipment as required.	P281
IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.	P304 + P340
Wash contaminated clothing before reuse.	P363
Store in a dry place. Store in a closed container.	P402 + P404
Store in a well-ventilated place. Keep cool.	P403 + P235
Store locked up.	P405
Dispose of contents/ container to an approved waste disposal plant.	P501

2.3 Other Hazards

Reacts violently with water	EUH014
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3. Composition / Information on Ingredients

3.1 Substances

Not applicable.

3.2 Mixtures

3.1.1 GHS Classification [EC: Regulation No 1272/2008; US: OSHA regulations]

Chemical Name	CAS #	EC No	EC Index No	REACH Reg No	Wt.%	Classification, Hazard Statement Codes
lithium tri-tert-butoxyaluminum hydride	17476-04-9	241-490-8	none	none	23-32	Water-react. 1 Skin Corr. 1B H260 H314
tetrahydrofuran	109-99-9	203-726-8	603-025-00-0	none	21-31	Flam. Liq. 2 Eye Irrit 2 Carc. 2 STOT SE 3 H225 H319 H351 H335
lithium di-tert-butoxyaluminum hydride (impruity)	24315-46-6	none	none	none	0-5	Water-react. 1 Skin Corr. 1B H260 H314
lithium tetra-tert-butoxyaluminum (impurity)	69537-16-2	none	none	none	0-5	Water-react. 1 Skin Corr. 1B H260 H314
tert-butyl alcohol	75-65-0	200-889-7	603-005-00-1	none	0-2	Flam. Liq. 2 Acute Tox. 4 Eye Irrit. 2 STOT SE 3 H225 H332 H319 H335

3.1.2 EC: Classification according to 67/548/EEC or 1999/45/EC [DSD/DPD]

Chemical Name	CAS #	EC No	Wt.%	Symbols	R-phrases
lithium tri-tert-butoxyaluminum hydride	17476-04-9	241-490-8	23-32	F; C;	R 14/15 R34
tetrahydrofuran	109-99-9	203-726-8	21-31	F; Carc. Cat. 3; Xi;	R11-19 R40 R36/37
lithium di-tert-butoxyaluminum hydride (impruity)	24315-46-6	none	0-5	F; C;	R 14/15 R34
lithium tetra-tert-butoxyaluminum (impurity)	69537-16-2	none	0-5	F; C;	R 14/15 R34
tert-butyl alcohol	75-65-0	200-889-7	0-2	F; Xn; Xi;	R11 R20 R36/37

(See Section 16 for R-phrase text)

4. First Aid Measures

4.1 Description of First Aid Measures

- EYES:** Immediately flush with water for at least 15 minutes, lifting the upper and lower eyelids intermittently. See a medical doctor or ophthalmologist immediately.
- SKIN:** Immediately flush with plenty of water while removing contaminated clothing and/or shoes, and thoroughly wash with soap and water. Obtain immediate medical attention. Contact a medical doctor if necessary.
- INGESTION:** Quickly wipe material from the mouth and rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. See a medical doctor immediately.
- INHALATION:** Remove to fresh air. If breathing discomfort occurs and persists, see a medical doctor. If breathing has stopped, give artificial respiration and see a medical doctor immediately.

4.2 Most Important Symptoms and effects, both acute and delayed

Symptoms of over-exposure will typically be a result of the corrosive nature of the substance with discomfort to skin and if swallowed, local effects with discomfort to the mouth and GI tract. Inhalation of solvent vapours may lead to dizziness and impairment of normal functions.

4.3 Indication of any immediate medical attention and special treatment needed.

Notes to medical doctor:

Product is highly alkaline and is corrosive to the eyes, skin and mucous membranes. Consideration should be given to careful endoscopy as stomach or esophageal burns, perforations or strictures may occur. Careful gastric lavage with an endotracheal tube in place should be considered. Observation may be warranted. Treatment is controlled removal of exposure followed by symptomatic and supportive care.

5. Fire-Fighting Measures

- 5.1 **Extinguishing media** DO NOT USE WATER OR CARBON DIOXIDE. Use dry chemical.
- 5.2 **Special hazards arising from the substance or mixture**
Hazardous combustion products Lithium hydroxide, aluminum oxide, aluminum hydroxide, carbon monoxide, and carbon dioxide.
General Hazard Flammable liquid. Lithium tri-t-butoxyaluminum hydride reacts with water, generating heat.
Properties contributing to
Flammability Water reactivity of product, and volatility of solvents.
Flashpoint Not available. The flashpoint of THF is -17°C
Flammable limits in air Not available. For tetrahydrofuran: Upper: 2% Lower: 11.8%
Auto ignition temperature Not available.
Sensitivity to static discharge Yes
Sensitivity to static impact Not applicable
- 5.3 **Advice for fire-fighters**
Wear full protective clothing and self-contained breathing apparatus (SCBA) approved for fire fighting. This is necessary to protect against the hazards of heat, products of combustion and oxygen deficiency. Do not breathe smoke, gases or vapors generated.

COMMENTS:

(See Section 10, Stability and Reactivity)

6. Accidental Release Measures

- 6.1 **Personal precautions, protective equipment and emergency procedures**
Before cleanup measures begin, review the entire SDS with particular attention to Section 2, Hazards Identification; and Section 8, Exposure Controls/Personal Protection. Remove all sources of ignition. Spilled material can catch fire spontaneously on contact with air, moisture, acids or oxidizing materials.
- 6.2 **Environmental precautions**
Contain spill. Do not wash into drains. Dispose of at qualified waste disposal facility.
- 6.3 **Methods and material for containment and cleaning up**
Remove all sources of ignition. Spilled material can catch fire spontaneously on contact with air, moisture, acids or oxidizing materials. Cover spill with dry extinguishant. DO NOT USE WATER OR CARBON DIOXIDE. Contain spill with absorbant. Expose to air until solvent has dissipated. Sweep up and place in approved transport container. Dispose of waste according to local and Federal laws and regulations.
- 6.4 **Reference to other sections**
Before cleanup measures begin, review the entire SDS with particular attention to Section 2, Hazards Identification; and Section 8, Exposure Controls/Personal Protection.
- 6.5 **Additional information**
Not specified.

7. Handling and Storage

- 7.1 **Precautions for safe handling**
KEEP AWAY FROM WATER, AIR AND OXIDIZING MATERIALS. Wear full face protection and gloves. Use in a closed system under argon or nitrogen.
- 7.2 **Conditions for safe storage, including any incompatibilities**
Keep away from heat, sparks and flame. Protect storage container from leaks and physical damage.
- 7.3 **Specific end use(s)**
For use only as a chemical intermediate under Strictly Controlled Conditions

8. Exposure Controls / Personal Protection

8.1 Control parameters

Note that DNELs and PNECs have not been derived for Lithium tri-tert-butoxyaluminum hydride as it is a strictly controlled transported intermediate

DNEL Tetrahydrofuran:

Long-term exposure, systemic, inhalation Not available
 Long-term exposure, systemic, dermal Not available

PNEC Tetrahydrofuran:

Not available

EXPOSURE LIMITS

<u>Chemical Name</u>	<u>EU</u>		<u>EH40 (UK WEL)</u>		<u>USA (ACGIH)</u>		<u>USA (OSHA)</u>	
	<u>TWA</u>	<u>STEL</u>	<u>TWA</u>	<u>STEL</u>	<u>TWA</u>	<u>STEL/Ceiling</u>	<u>PEL</u>	<u>STEL/Ceiling</u>
tetrahydrofuran		100 ppm	50 ppm	100 ppm	50 ppm	100 ppm	200 ppm	
t-butanol	none		100 ppm	150 ppm	100 ppm		none	

8.2 Exposure controls

Engineering controls:

Use in closed system under argon or nitrogen. If personal contact can occur, use local exhaust ventilation (explosion-proof), to keep airborne concentrations below exposure limits.

Personal protective equipment

Eyes and Face:

Chemical splash goggles with a face shield.

Respiratory:

Wear a respirator approved for protection against organic vapours and mists when adequate ventilation is not available
 US: NIOSH or MSHA approved
 Europe: CEN Class A type

Protective Clothing:

Gloves: Nitrile (typical permeation breakthrough time >480 minutes)
 These glove recommendations should not be used as the absolute basis for glove selection. Actual in-use conditions may vary glove performance from the controlled conditions of laboratory tests. Factors such as concentration and temperature, glove thickness and glove reuse, may affect performance. Other glove requirements, such as length, dexterity, cut, abrasion, puncture and snag resistance, or glove grip need to be considered in making your final selection. For flammable products, the recommended gloves provide chemical but not fire protection

Other: Rubber clothing.

Work Hygienic

Quick-drench eyewash and safety shower.

Practices:

9. Physical and Chemical Properties

9.1 Information on basic physical and chemical properties

Appearance:

Clear to slightly hazy liquid, colorless to light gray/yellow

Odor:

Pungent

Odor threshold:

Not available

pH:

Reacts exothermically with water giving mixture with pH >12

Melting point:

Not available. Tetrahydrofuran freezes at -108.44 °C

Boiling point:

Not available. The boiling point of tetrahydrofuran is 65.00 °C

Flashpoint

Not available. The flashpoint of THF is -17°C

Evaporation rate(butyl acetate = 1):

Not available

Flammability:

Water reactive material in flammable liquid solvent

Flammable limits:

Not applicable for formulation. For tetrahydrofuran: Upper: 2% Lower: 11.8%

Vapor pressure:

162.1 mm Hg at 20 °C (tetrahydrofuran)

Vapor density (air = 1):

2.49 (tetrahydrofuran)

Specific gravity:

0.89 g/ml

<u>Solubility in water:</u>	Reacts exothermically with water
<u>Partition coefficient n-octanol/ water:</u>	Not available
<u>Autoignition temperature:</u>	Not available
<u>Decomposition temperature:</u>	Not available
<u>Viscosity:</u>	Not available
<u>Explosive properties:</u>	Not explosive
<u>Oxidizing properties:</u>	Not an oxidizer
9.2 <u>Other information</u>	
<u>Self-reactive properties</u>	Does not meet classification criteria.
<u>Pyrophoric properties</u>	Does not meet classification criteria.
<u>Self-heating properties</u>	Does not meet classification criteria.
<u>Water reactive properties</u>	Water reactive; Category 1
<u>Corrosive to metals</u>	Does not meet classification criteria.
<u>Molecular weight:</u>	254.26 (lithium tri-tert-butoxyaluminum hydride)

10. Stability and Reactivity

10.1 <u>Reactivity</u>	Reactive with water and damp air
10.2 <u>Chemical stability</u>	Stable if kept away from air and moisture.
10.3 <u>Possibility of hazardous reaction</u>	Reaction with water, air, oxidizers, acids to form hydrogen, lithium hydroxide, aluminum hydroxide/oxide, and t-butanol.
10.4 <u>Conditions to avoid</u>	Open air. Heat, sparks or flames
10.5 <u>Incompatible materials</u>	Heat, fire, air, water, acids and oxidizing chemicals
10.6 <u>Hazardous decomposition products</u>	Lithium oxide, lithium hydroxide, hydrogen, aluminum oxide, and aluminum hydroxide

11. Toxicological Information

11.1 Information on toxicological effects

The mixture has not been tested, but properties can be predicted based on the properties of the two components

(a) acute toxicity	Lithium tri-tert-butoxyaluminum hydride: Corrosive Classified as acute toxicity category 4 based on component data and hydrolysis products: t-Butanol (hydrolysis product) Acute toxicity Category 4 oral and inhalation
(b) skin corrosion/irritation	Classified as corrosive on the basis of lithium tri-tert-butoxyaluminum hydride.
(c) serious eye damage/irritation	Classified as corrosive on the basis of lithium tri-tert-butoxyaluminum hydride.
(d) respiratory/skin sensitisation	No components are considered to be potential sensitizing agents.
(e) germ cell mutagenicity	None of the components considered to be mutagenic.
(f) carcinogenicity	Classified as a carcinogen, category 2, based on tetrahydrofuran.
(g) reproductive toxicity	No components are considered to be reproductive toxins.
(h) STOT-single exposure	Classified as STOT single exposure, category 3 due to tetrahydrofuran.
(i) STOT-repeated exposure	No components are considered to be STOT-repeat exposure.
(j) aspiration hazard	No components are considered to be aspiration toxicity, Category 1.

Acute Effects From Overexposure:

This product is corrosive to the eyes, skin, mucous membranes, upper respiratory tract, and is water reactive. Inhalation of vapors may cause dizziness, nausea, anesthesia, numbness, burning sensation and motor weakness in fingers and toes, incoordination, and headache. May cause peripheral nervous system disorder and/or damage.

Chronic Effects From Overexposure:

No data available for the product.

Tetrahydrofuran: Repeated or prolonged exposure may cause signs of central nervous system depression and respiratory irritation. Tetrahydrofuran is listed by NTP as a substance that is reasonably anticipated to be a carcinogen. THF gave negative results in bacterial mutagenicity tests with and without metabolic activation. One animal study suggests that THF does not cause effects at doses which are not maternally toxic.

Carcinogenicity Listings

Eh40: Tetrahydrofuran is listed.
IARC: Tetrahydrofuran is listed
NTP: Tetrahydrofuran is listed.
OSHA: Not listed.
ACGIH: Tetrahydrofuran is listed.

12. Ecological Information

12.1 Toxicity:

The mixture has not been tested, but properties can be predicted based on the properties of the components

Tetrahydrofuran:

48 hr. LC₅₀ = 2820; 2930 mg/l (orfe) [Handbook Env. Data on Org. Chem., 4th Ed]

96 hr. LC₅₀ = 2160 mg/L (fathead minnow) [Handbook Env. Data on Org. Chem., 4th Ed]

12.2 Persistence and degradability

Lithium tri-tert-butoxyaluminum hydride: Lithium tri-tert-butoxyaluminum hydride reacts exothermically with water. Hydrolysis products consist of lithium hydroxide, t-butanol, hydrogen gas and aluminum hydroxide/oxide

Tetrahydrofuran: Tetrahydrofuran is expected to volatilize from both water and soil and leach into groundwater. It will not photodegrade or adsorb to sediment. Limited evidence suggests it may biodegrade. Based on a relatively low Kow (0.47), it is not expected to bioconcentrate.

12.3 Bioaccumulative potential

Not available.

12.4 Mobility in soil

Solvents not expected to be mobile.

12.5 Results of PBT and vPvB assessment

Not available

12.6 Other adverse effects

Due to the nature of the material and the specialist applications, this product is not considered to be a risk to the environment.

13. Disposal Considerations

13.1 Waste treatment methods

Disposal method:

Do not discharge to waste water systems.

Spent solvent may be sent for recovery or used as fuel if permitted under local regulations

Dispose of waste according to local and national laws and regulations.

14. Transport Information

14.1 UN Number

UN3399

14.2 UN proper shipping name (IMDG, ICAO, ADR, DOT)

Organometallic substance, liquid, water-reactive, flammable (Tri-tert-butoxyaluminum lithium hydride solution in tetrahydrofuran)

14.3 Transport hazard class(es) (IMDG, ICAO, ADR, DOT)

Dangerous when wet, 4.3 (3, Flammable liquid)

14.4 Packing group (IMDG, ICAO, ADR, DOT)

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14.5 Environmental hazards

None

14.6 Special precautions for user

None

14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

None

15. Regulatory Information

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

EUROPEAN UNION:

German Wassergefährdungsklasse (water hazard class)

lithium tri-tert-butoxyaluminum hydride	1
tetrahydrofuran	1
t-butanol	1

UNITED STATES:

Section 311 Hazard Category (40 CFR 370):

Fire hazard, immediate (acute) health hazard, reactive

Section 313 Reportable Ingredients (40 CFR 372):

This product contains t-butanol, which is a substance subject to the reporting requirements of Section 313 of the Emergency Planning and Community Right-to-Know act of 1986 and 40 CFR 372.

This information must be included in all MSDS's that are copied and distributed for this material.

Not listed

Section 302 Extremely Hazardous Substances (40 CFR 355):

CERCLA Hazardous Substance (40 CFR 302.4):

Tetrahydrofuran is listed. The reportable quantity is 1000 lbs.

TSCA Sec 12b Export Notification:

This product is subject to TSCA 12(b) Export Notification requirements due to the presence of tetrahydrofuran.

Health: 3 Flammability: 3 Reactivity: 2 Special: ~~W~~

NFPA Rating:

INTERNATIONAL INVENTORY STATUS:

Inventory/Country

Product Status

EINECS (EU)	Listed
TSCA (US)	Listed
ECL (Korea)	Listed
DSL (Canada)	Not listed. Lithium tri-t-butoxyaluminum hydride is on the NDSL

15.2 Chemical Safety Assessment

Not available.

16. Other Information

European Union:

R Phrases:

Highly flammable	R11
Reacts violently with water, liberating extremely flammable gases	R14/15
May form explosive peroxides	R19
Harmful by inhalation	R20
Causes burns	R34
Irritating to eyes and respiratory system	R36/37
Irritating to respiratory system	R37
Limited evidence of a carcinogenic effect	R40

List of Abbreviations used in this SDS:

PBT	Persistent, Bioaccumulative and Toxic
vPvB	very Persistent, very Bioaccumulative
PEC	Predicted environmental concentration
PNEC	Predicted no effect concentration
DNEL	Derived no effect level

Specific uses identified for Exposure Scenarios

Not available

REVISION SUMMARY: Revision # 0. All new SDS.

This SDS has been prepared to meet U. S. OSHA Hazard Communication Standard requirements.
type 2d

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