



***t*-BUTYLLITHIUM IN HEPTANE**

CAS No. 594-19-4

Product Names *t*-Butyllithium, *t*-BuLi, TBL

Formula (CH₃)₃C-Li

Appearance Clear, yellowish solution

Application This formulation of *t*-Butyllithium in Heptane, while still pyrophoric, has a significantly higher flash point than the traditional pentane formulation. TBL is particularly useful in lithium-halogen exchange reactions. TBL can be used as a strong base in organic synthesis. TBL is more reactive than the *t*-butyl Grignard reagent in nucleophilic additions to carbonyl and nitrile substrates. TBL is also useful in the displacement of halide or alkoxide ligands of inorganic compounds, such as Phosphorus, Silicon, Tin, and Titanium. References: *The Chemistry of Organolithium Compounds*, ed. Zvi Rappoport and Ilan Marek, Wiley, 2004, West Sussex, England.

Product Specification

Typical*

<i>t</i> -Butyllithium, wt %	23 – 31
Free Alkalinity, wt %	0.8 max

* This product can be made to agreed upon customer specifications.

Solvent Heptane

Physical Properties	Molecular weight	64.06
	Density @20°C	0.69 g/ml (5.76 lb/gal)
	Contained <i>t</i> -Butyllithium	110 g/L (0.92 lb/gal)
	Pyrophoricity	Pyrophoric

Solubility In the pure state, *t*-butyllithium is a solid. *t*-Butyllithium is very soluble in aliphatic, aromatic and ethereal solvents; however it will react with the latter two solvent types even at 0°C.

Thermal Stability At 15°C and 40°C, the average decomposition rates were 0.02 and 0.1 wt. % per day, respectively. Recommended storage: 15°C for a maximum of 150 days and preferably at 0°C.



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Toxicity/Safety Data Pyrophoric liquid. Can catch fire if exposed to air. Reacts violently with water to give off flammable gases and corrosive dusts. Corrosive to eyes (may cause blindness), skin, nose, throat and stomach. Can catch fire on contact with body moisture or if exposed to air. Inhalation of vapors may cause dizziness, nausea, anesthesia, numbness, motor weakness in fingers and toes, incoordination, and headache. If ingested, may produce a lung aspiration hazard.

COMPLETE INFORMATION ON TOXICITY AND SAFETY IS CONTAINED IN THE OPTIMA MATERIAL SAFETY DATA SHEET (MSDS) AVAILABLE FOR THIS PRODUCT.

Handling/Storage/Disposal Keep away from water, air, and oxidizing materials. Wear full face protection and gloves. Use in a closed system under argon or nitrogen. Keep away from heat, sparks and flame. Protect storage container from leaks and physical damage.

Shipping Containers	Bulk containers	2500 – 20000 L
	Cylinders	#5 – 420 L
	Glass bottles	125 mL, 500 mL, and 1 L

Shipping Limitations Shipments of TBL are described as " Organometallic substance, liquid, pyrophoric, water-reactive (*T-BUTYLLITHIUM, HYDROCARBON SOLUTION*), 4.2 (4.3), UN 3394, PG I". Shipments require "Spontaneously Combustible" and "Dangerous When Wet" labels.

Post, Parcel, Air	Not acceptable
Sea	Class 4.2 (4.3) (IMDG)
Road, Rail (USA)	Class 4.2 (4.3) (DOT)
Road, Rail (EU)	Class 4.2 (4.3) (RID/ADR)

For shipments within Europe, labeling for supply requirements are:

F	Highly Flammable
C	Corrosive
N	Hazardous for the Environment
R&S phrases	See Material Safety Data Sheet

Responsible Care[®] initiative dictates that all shipments of lithium chemicals must be transported in a DOT-approved vehicle in a responsible manner (i.e., no flat bed trucks).

Additional Resources Refer to the Butyllithium Safe Handling Guide available on-line at www.optimachem.com.