



n-HEXYLLITHIUM 33% IN HEXANES (HxLi)

CAS No. 21369-64-2

QS-PDS-019 Revision: 01

Product Names *n*-Hexyllithium, HxLi, NHL

Formula CH₃(CH₂)₄-Li

Appearance Clear, colorless to yellow solution

Application *n*-Hexyllithium is a *non-pyrophoric* strong base, primarily used in organic synthesis in deprotonation reactions and as a lithiation reagent. The advantage of this reagent is that the by-product of a deprotonation reaction is *n*-hexanes. *n*-Hexanes is less volatile and has a higher flash point than the *n*-butane generated from a deprotonation with *n*-butyllithium. 1) *The Chemistry of Organolithium Compounds*; Pergamon: Oxford, **1974**; 2) *Organolithium Methods*; Academic Press: London, **1988**.

Product Specification	<i>n</i> -Hexyllithium, wt%	<u>Guaranteed</u> 30.0 – 34.0
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*This product can be made to agreed upon customer specifications.

Solvent Commercial hexanes

Physical Properties	Molecular weight	92.10
	Density @20°C	0.705g/mL (5.88 lb/gal)
	Contained hexyllithium	232.7 g/L (1.94 lb/gal)
	Pyrophoricity	Non-pyrophoric

Solubility *n*-Hexyllithium is miscible in all proportions with aliphatic, aromatic, and ethereal solvents; however, there is some reactivity with the latter two solvent types.

Thermal Stability At 20°C, the average decomposition rate is <0.002 wt.% per day. Recommended storage: 20°C or lower.



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Toxicity/Safety Data Flammable liquid. Water reactive. In case of fire, do not use water or carbon dioxide. Reacts violently with water to give off flammable gases, and corrosive dusts. Clear yellowish liquid, gasoline-like odor. Corrosive to the eyes (may cause blindness), skin, nose and throat. Inhalation of vapors may cause dizziness, nausea, anesthesia, numbness, burning sensation and motor weakness in fingers and toes, incoordination, 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 Use in a closed system under argon or nitrogen. Do not get in eyes, on skin or clothing. Do not breathe vapors or mist. Store in a cool place. Keep container closed. Keep away from sources of ignition, water air, acids and oxidizing agents.

Shipping Containers	Bulk containers	2000 – 20000 L
	Cylinders	#5 – 420 L
	Glass bottles	125 mL, 500 mL, and 1L

Shipping Limitations Shipments of NHL are described as "Corrosive Liquid, Flammable, N.O.S., (HEXYLLITHIUM IN HEXANES), 8 (3), UN2920, PG I." Shipments require "Corrosive" and "Flammable Liquid" labels.

Post, Parcel	Not acceptable
Sea	Class 8 (3) (IMDG)
Road, Rail (USA)	Class 8 (3) (DOT)
Road, Rail (EU)	Class 8 (3) (RID/ADR)
Air	Class 8 (3) (IATA)
	1.0 L maximum per inner glass container.
	2.5 L maximum per single/outer container.
	Cargo aircraft only.

For shipments within Europe, labeling for supply requirements are:

F	Highly Flammable
C	Corrosive
N	Dangerous 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 Organometallics and Reactive Specialty Organics Safe Handling Guide.