



PHENYLITHIUM 18.5% IN DBE (PhLi)

CAS No. 591-51-5

QS-PDS-020 Revision: 01

Product Names Phenyllithium, PhLi

Formula C₆H₅-Li

Appearance Amber to black solution

Application This patented (U. S. Patent 5,626,798) formulation of phenyllithium in dibutyl ether is non-pyrophoric and does *not* contain highly flammable diethyl ether. PhLi is particularly useful in lithium-halogen exchange reactions of aromatic heterocycles. PhLi can be used as a strong base, in organic synthesis, but generates benzene. It has been employed for the generation of ylides and benzyne. PhLi is more reactive than the phenyl Grignard reagent in nucleophilic additions to carbonyl and nitrile substrates. It is also useful in halide or alkoxide substitution/displacement reactions of inorganic compounds, such as phosphorus, silicon, tin and titanium. *J. Organomet. Chem.* **1988**, 342, 143 and references therein.

Product Specification

Guaranteed*

Phenyllithium, wt%	17 – 24
Di- <i>n</i> -butyl ether, wt%	75 – 81
Biphenyl, wt%	2.0

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

Solvent Di-*n*-butyl ether (DBE)

Physical Properties	Molecular weight	84.05
	Density @15°C	0.83g/mL (6.92 lb/gal)
	Contained PhLi	153.5g/L (1.28 lb/gal)
	Pyrophoricity	Non-pyrophoric

Solubility Soluble up to ~30 wt% at 20°C

Thermal Stability At 20°C and 40°C, the average decomposition rates were 0.22 and 0.39 wt.% per day, respectively. Recommended storage: 10°C for a maximum of 150 days.



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Toxicity/Safety Data Flammable liquid. Corrosive to eyes (may cause blindness), skin, nose and throat. Contains benzene, a known carcinogen.

ADDITIONAL INFORMATION ON SAFETY IS CONTAINED IN THE OPTIMA NEW PRODUCT DATA SHEET (NPDS) 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 inert atmosphere of argon or nitrogen. Keep away from sources of ignition, water air, acids and oxidizing agents. Do not get in eyes, on skin, or on clothing. Protect storage container against leaks and physical damage.

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

Shipping Limitations Shipments of PhLi are described as "Flammable Liquid, Corrosive, N.O.S., (PHENYLLITHIUM IN DIBUTYL ETHER), 3 (8), UN2924, PG II." Shipments require "Flammable Liquid" and "Corrosive" labels.

Post, Parcel	Not acceptable
Sea	Class 3 (8) (IMDG)
Road, Rail (USA)	Class 3 (8) (DOT)
Road, Rail (EU)	Class 3 (8) (RID/ADR)
Air	Class 3 (8) (IATA)
	2.5 L maximum per inner glass container.
	5.0 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.