Methyllithium (MeLi-9307)  
CAS No. 917-54-4

Product Names: Methyllithium, Methyllithium 9307, MeLi

Formula: CH₃–Li

Appearance: Colorless to light yellow solution

Application: MeLi is a patented (U. S. Patent 4,976,886) formulation of methyllithium in THF/cumene that is non-pyrophoric and does not contain highly flammable diethyl ether. The product is stabilized through the addition of magnesium to yield a molar ratio of Li:Mg of 93:07. The presence of magnesium increases solubility and greatly reduces the rate of thermal decomposition, which can lead to the build-up of methane gas pressure. MeLi can be used for methylation via 1,2 addition to carbonyl or nitrile compounds. It is also useful in the preparation of vitamin and steroid derivatives, in carbene-type reactions in the formation of allenes and alkoxyalkanopanes, and in metation reactions in the preparation of halogenated alkynyllithiums and steroidal alkynyl compounds. It can be used in the reduction of certain transition metal halides [e.g., PdCl₂ to Pd (0)], in the preparation of lithium methyl cuprates for 1,4-conjugate addition, and to prepare other organometallics [e.g., Me₂Mg, MeTi(NE₂)₃, Me₃Al, Me₃As, Me₃In or Me₃Ga].

Product Specification

<table>
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<th>Guaranteed*</th>
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<td>Methyllithium, wt%</td>
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* This product can be made to agreed upon customer specifications.

Solvent:
- THF, wt.%: 15
- Cumene, wt.%: 82

Physical Properties:
- Molecular weight: 21.97
- Density @20°C: 0.86g/mL (7.18 lb/gal)
- Contained MeLi: 24.9g/L (0.21 lb/gal)
- Pyrophoricity: Non-pyrophoric

Solubility: The solubility of methyllithium at >15ºC is 1.3 M; however, at 0ºC, the solubility is 0.9 M. At <0ºC, MeLi precipitates as large MeLi•THF crystals which redissolve on warming and with agitation.

Thermal Stability: At 15ºC and 40ºC, the average decomposition rates were 0.008 and 0.09 wt. % per day, respectively. Recommended storage: 10ºC for a maximum of 60 days and 0ºC for 3-6 months. At 40ºC, a slight pressure develops in containers and the product color changes to dark orange. MeLi degrades by metation of the aromatic solvent to afford methane gas and cumyllithiums.
METHYLLITHIUM (MeLi-9307)  
CAS No. 917-54-4

Toxicity/Safety Data
Flammable liquid. Water reactive. In case of fire do not use water or carbon dioxide. Corrosive to eyes (may cause blindness), skin, respiratory tract, mucous membranes. 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
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

Shipping Limitations
Shipments of MeLi are described as "Flammable Liquid, Corrosive, N.O.S., (METHYLLITHIUM 9307 IN TETRAHYDROFURAN/CUMENE), 3 (8), UN2924, PGII." Shipments require "Flammable Liquid" and "Corrosive" labels.

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<tr>
<th>Post, Parcel</th>
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<tbody>
<tr>
<td>Sea</td>
<td>Class 3 (8) (IMDG)</td>
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<td>Road, Rail (USA)</td>
<td>Class 3 (8) (DOT)</td>
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<tr>
<td>Road, Rail (EU)</td>
<td>Class 3 (8) (RID/ADR)</td>
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<tr>
<td>Air</td>
<td>Class 3 (8) (IATA)</td>
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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.