

Product Data Sheet

Product Name: Lithium aluminum deuteride

Cat. No.: GD15777

Chemical Properties

Cas. No. 14128-54-2

Formula LiAlD₄

M.Wt 41.98

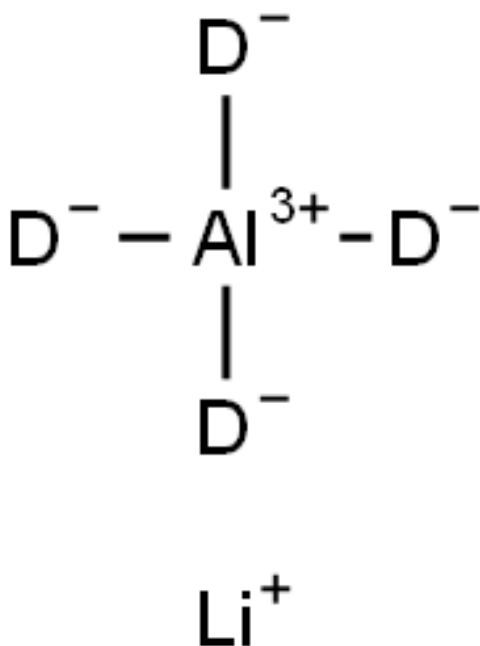
Solubility

Storage Store at 2-8°C, protect from light

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Protocol

Protocol for [13CD₂ 15N]-C-Benzo[b]thiophen-3-yl-methylamine 6 Synthesis^[1]:

1. Add lithium aluminum deuteride (1.0M THF solution; 4.0mL; 4.0mmol) in anhydrous diethyl ether (10mL), [13C15N]benzo[b]thiophene-3-carbonitrile (322.4mg, 2.0 mmol) in anhydrous diethyl ether (6mL) at room temperature dropwise.

Caution: Product has not been fully validated for medical applications. For research use only.

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2. Stir and heat the reaction mixture in an oil bath to reflux for 3h and then cool into an ice-water bath and quenched by addition of a pH=7.0 buffer solution (20mL).
3. Separate the organic layer and extract the aqueous layer three times with dichloromethane.
4. Combine the organic layers and dry over MgSO_4 , filter, and evaporate the solvents on a rotary evaporator to give an oil residue.
5. Dissolve the oil residue in a small amount of dichloromethane and subject to chromatography on Biotage Horizon system with silica gel column eluted with 10% methanol in dichloromethane containing about 1% of ammonium hydroxide.
6. Collect and combine fractions containing product, and remove the solvents on a rotary evaporator to give the desired compound as yellowish oil (185.5mg, 55%).

*This protocol only provides a guideline for lithium aluminum deuteride, and should be modified according to your specific needs

References:

[1] Lin, Ronghui et al. "Expeditious syntheses of stable and radioactive isotope-labeled anticonvulsant agent, JNJ-26990990, and its metabolites." Journal of labelled compounds & radiopharmaceuticals vol. 56,1 (2013): 22-6. doi:10.1002/jlcr.3013

Background

Lithium aluminum deuteride is a material applied in isotype labeling, deuterium exchange reactions, deuterium isotope effects, substrate for chemical synthesis (including organometallic compounds).

In isotype labeling, lithium aluminum deuteride (1.0M THF solution; 4.0mL; 4.0mmol) reduce $[^{13}\text{C}^{15}\text{N}]$ benzo[b]thiophene-3-carbonitrile to give $[^{13}\text{CD}_2^{15}\text{N}]$ benzo[b]thiophen-3-yl-methylamine stable isotope-labeled compound with four stable isotope atoms^[1]. Lithium aluminum deuteride is also used for novel cage oxaheterocycles synthesis (155mg, 4.08mmol in dry THF (20mL)) and deuterium-labeled analogs of the lipid hydroperoxide-derived bifunctional electrophile 4-oxo-2(*E*)-nonenal synthesis as a deuteride donor^[2,3]. The role of lithium aluminum deuteride in the selective deuteration of carbonyl-containing molecules aids in elucidating reaction mechanisms and metabolic pathways.

References:

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[2] Marchand, A P et al. "Synthesis of novel cage oxaheterocycles." *The Journal of organic chemistry* vol. 66,6 (2001): 2072-7. doi:10.1021/jo001611c

[3] Arora, Jasbir S et al. "Synthesis of deuterium-labeled analogs of the lipid hydroperoxide-derived bifunctional electrophile 4-oxo-2(*E*)-nonenal." *Journal of labelled compounds & radiopharmaceuticals* vol. 54,5 (2011): 247-251. doi:10.1002/jlcr.1860

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