SCREENING-LEVEL HAZARD CHARACTERIZATION

Butyllithium
(CASRN 109-72-8)

The High Production Volume (HPV) Challenge Program[1] was conceived as a voluntary initiative aimed at developing and making publicly available screening-level health and environmental effects information on chemicals manufactured in or imported into the United States in quantities greater than one million pounds per year. In the Challenge Program, producers and importers of HPV chemicals voluntarily sponsored chemicals; sponsorship entailed the identification and initial assessment of the adequacy of existing toxicity data/information, conducting new testing if adequate data did not exist, and making both new and existing data and information available to the public. Each complete data submission contains data on 18 internationally agreed to "SIDS" (Screening Information Data Set[1,2]) endpoints that are screening-level indicators of potential hazards (toxicity) for humans or the environment.

The Environmental Protection Agency's Office of Pollution Prevention and Toxics (OPPT) is evaluating the data submitted in the HPV Challenge Program on approximately 1400 sponsored chemicals by developing hazard characterizations (HCs). These HCs consist of an evaluation of the quality and completeness of the data set provided in the Challenge Program submissions. They are not intended to be definitive statements regarding the possibility of unreasonable risk of injury to health or the environment.

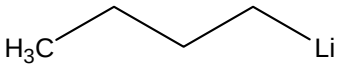
The evaluation is performed according to established EPA guidance[2,3] and is based primarily on hazard data provided by sponsors; however, in preparing the hazard characterization, EPA considered its own comments and public comments on the original submission as well as the sponsor's responses to comments and revisions made to the submission. In order to determine whether any new hazard information was developed since the time of the HPV submission, a search of the following databases was made from one year prior to the date of the HPV Challenge submission to the present: (ChemID to locate available data sources including Medline/PubMed, Toxline, HSDB, IRIS, NTP, ATSDR, IARC, EXTOXNET, EPA SRS, etc.), STN/CAS online databases (Registry file for locators, ChemAbs for toxicology data, RTECS, Merck, etc.) and Science Direct. OPPT's focus on these specific sources is based on their being of high quality, highly relevant to hazard characterization, and publicly available.

OPPT does not develop HCs for those HPV chemicals which have already been assessed internationally through the HPV program of the Organization for Economic Cooperation and Development (OECD) and for which Screening Initial Data Set (SIDS) Initial Assessment Reports (SIAR) and SIDS Initial Assessment Profiles (SIAP) are available. These documents are presented in an international forum that involves review and endorsement by governmental

[1] U.S. EPA. High Production Volume (HPV) Challenge Program; http://www.epa.gov/chemrtk/index.htm.
[2] U.S. EPA. HPV Challenge Program – Information Sources; http://www.epa.gov/chemrtk/pubs/general/guidocs.htm.
[3] U.S. EPA. Risk Assessment Guidelines; http://cfpub.epa.gov/ncea/raf/rafguid.cfm.

authorities around the world. OPPT is an active participant in these meetings and accepts these documents as reliable screening-level hazard assessments.

These hazard characterizations are technical documents intended to inform subsequent decisions and actions by OPPT. Accordingly, the documents are not written with the goal of informing the general public. However, they do provide a vehicle for public access to a concise assessment of the raw technical data on HPV chemicals and provide information previously not readily available to the public.

Chemical Abstract Service Registry Number (CASRN)	**109-72-8**
Chemical Abstract Index Name	Lithium, butyl-
Structural Formula	

Summary

This chemical is a liquid in pure form and is formulated in dilute hydrocarbon solvent and stored in sealed systems under an inert gas. It reacts violently with air or water and, therefore, meaningful measurements of its vapor pressure and water solubility properties cannot be made. If released to the environment, this chemical would decompose rapidly to form lithium hydroxide and butane. Due to the highly reactive nature of this substance, it is judged to have low persistence (P1) and low bioaccumulation potential (B1).

No mammalian and aquatic toxicity data are available. Due to the known reactivity, testing this highly reactive chemical would not generate meaningful data.

The sponsor, FMC Corporation, submitted a Test Plan and Robust Summaries to EPA for butyllithium (CAS No. 109-72-8; 9th CI name: lithium, butyl-) on March 8, 2002. EPA posted the submission on the ChemRTK HPV Challenge website on April 2, 2002 (http://www.epa.gov/chemrtk/pubs/summaries/butylith/c13633tc.htm). EPA comments on the original submission were posted to the website on August 22, 2002. Public comments were also received and posted to the website.

1. Chemical Identity

1.1 Identification and Purity

The HPV submission for this chemical did not include information on identification and purity in the Test Plan (2002).

1.2 Physical-Chemical Properties

The physical-chemical properties of the butyllithium are summarized in Table 1. Due to this substance's highly reactive nature in air and water, vapor pressure, water solubility and partition coefficient properties cannot be measured.

Table 1. Physical-Chemical Properties of Butyllithium[1]

Property	Value
CASRN	109-72-8
Molecular Weight	64.1
Physical State	Liquid in pure form
Melting Point	<0°C; -76°C (measured)[2]
Boiling Point	150°C with decomposition (measured)[3]; 80–90°C at 0.0001 mm Hg (measured)[4]
Vapor Pressure	4.4×10^{-4} mm Hg at 60°C (measured)[5]
Water Solubility	Not applicable (reacts violently when exposed to water)
Dissociation Constant (pK_a)	Not applicable (reacts violently when exposed to water)
Henry's Law Constant	Not applicable (reacts violently when exposed to water)
Log K_{ow}	Not applicable (reacts violently when exposed to water)

[1]FMC Corporation Lithium Division. March 11, 2002. Robust Summary and Test Plan for Butyllithium. http://www.epa.gov/chemrtk/pubs/summaries/butylith/c13633tc.htm.
[2]Gerhartz, W. (ed.). 1990. Ullmann's Encyclopedia of Industrial Chemistry. 5th ed. Volume A15. p. 411. Deerfield Beach, FL: VCH Publishers.
[3]Ashford, R.D. 1994. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., p. 157.
[4]Lewis, R.J. 1999. Sax's Dangerous Properties of Industrial Materials. 10th ed. Volumes 1–3. p. 641. New York, NY: John Wiley & Sons Inc.
[5]Kirk-Othmer Encyclopedia of Chemical Technology. 1995. 4th ed. Volumes 1 to present. New York, NY: John Wiley and Sons, Inc., v. 15, p. 454.

2. General Information on Exposure

2.1 Production Volume and Use Pattern

This chemical had an aggregated production and/or import volume in the United States during calendar year 2005 between 1 million to 10 million pounds. Non-confidential information in the IUR indicates that the industrial processing and uses of this chemical include process regulators, used in vulcanization or polymerization processes. The HPV submission for butyllithium states that the chemical is used as an initiator for polymerization in the production of automobile tires, and has specialized applications in the synthesis of pharmaceuticals.

2.2 Environmental Exposure and Fate

No quantitative information is available of release of this chemical to the environment.

The environmental fate properties are provided in Table 2. If released to the environment, butyllithium would decompose rapidly to form lithium hydroxide and butane. Therefore, fate processes such as volatilization, mobility in soil, and biodegradation are not relevant environmental fate properties. Due to butyllithium's highly reactive nature, it is unlikely that meaningful, measurements of its vapor pressure, water solubility and partition coefficient properties can be made. Butyllithium is judged to have a low persistence (P1) and low bioaccumulation potential (B1).

Table 2. Environmental Fate Characteristics of Butyllithium[1]

Property	**Value**
Photodegradation Half-life	Not applicable (reacts violently when exposed to air or water)
Hydrolysis Half-life	Unstable in water with immediate decomposition
Biodegradation	Not applicable (reacts violently when exposed to air or water)
Bioconcentration	Not applicable (reacts violently when exposed to air or water)
Log K_{oc}	Not applicable (reacts violently when exposed to air or water)
Fugacity (Level III Model)	Not applicable (reacts violently when exposed to air or water)
Persistence[2]	P1 (low)
Bioaccumulation[2]	B1 (low)

[1]FMC Corporation Lithium Division. March 11, 2002. Robust Summary and Test Plan for Butyllithium. http://www.epa.gov/chemrtk/pubs/summaries/butylith/c13633tc.htm.
[2]Federal Register. 1999. Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances. *Federal Register* 64, Number 213 (November 4, 1999) pp. 60194–60204.

Conclusion: Butyllithium is a liquid in pure form and is formulated in dilute hydrocarbon solvent and stored in sealed systems under an inert gas. It reacts violently with air or water and, therefore, meaningful measurements of its vapor pressure and water solubility properties cannot be made. If released to the environment, butyllithium would decompose rapidly to form lithium hydroxide and butane. Due to the highly reactive nature of this substance, butyllithium is judged to have low persistence (P1) and low bioaccumulation potential (B1). Partial physical-chemical properties were provided, however, the environmental fate of butyllithium was identified as a data gap under the HPV Challenge Program.

3. Human Health Hazard & Hazard to the Environment

No mammalian and aquatic toxicity data are available. Due to the known reactivity, testing this highly reactive chemical would not generate meaningful data.