SAFETY DATA SHEET

Version 8.9
Revision Date 04/28/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Isopropyllithium solution

Product Number : 529745
Brand : Aldrich

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids : Category 1

Skin irritation : Category 2

Serious eye damage : Category 1

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Specific target organ toxicity - single exposure	:	Category 3 (Central nervous system)
Aspiration hazard	:	Category 1
Short-term (acute) aquatic hazard	:	Category 2
Long-term (chronic) aquatic hazard	:	Category 2

Other hazards

None known.

GHS label elements

Hazard pictograms :

Signal Word : Danger

Hazard Statements :
H224 Extremely flammable liquid and vapor.
H304 May be fatal if swallowed and enters airways.
H315 Causes skin irritation.
H318 Causes serious eye damage.
H336 May cause drowsiness or dizziness.
H411 Toxic to aquatic life with long lasting effects.

Precautionary Statements :

Prevention:

P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242 Use only non-sparking tools.
P243 Take precautionary measures against static discharge.
P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.
P280 Wear protective gloves/ eye protection/ face protection.

Response:

P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.

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P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P331 Do NOT induce vomiting.
P332 + P313 If skin irritation occurs: Get medical advice/ attention.
P362 Take off contaminated clothing and wash before reuse.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391 Collect spillage.

Storage:

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P403 + P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Mixture

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
pentane	109-66-0*	>= 90 - <= 100	-
isopropyllithium	1888-75-1*	>= 1 - < 5	-

* Indicates that the identifier is a CAS No.
Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this material safety data sheet to the doctor in attendance.
If inhaled : After inhalation: fresh air. Call in physician.

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In case of skin contact	:	In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.
In case of eye contact	:	After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.
If swallowed	:	After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.
Most important symptoms and effects, both acute and delayed	:	The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11
Protection of first-aiders	:	For personal protection see section 8.
Notes to physician	:	No data available

SECTION 5. FIRE-FIGHTING MEASURES

Suitable extinguishing media	:	Foam Carbon dioxide (CO2) Dry powder
Unsuitable extinguishing media	:	For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	:	Combustible. Pay attention to flashback. Vapors are heavier than air and may spread along floors. Development of hazardous combustion gases or vapours possible in the event of fire. Forms explosive mixtures with air at ambient temperatures.

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Hazardous combustion products	:	Carbon oxides Lithium oxides
Specific extinguishing methods	:	No data available
Further information	:	Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	:	Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	:	Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	:	Do not let product enter drains. Risk of explosion.
Methods and materials for containment and cleaning up	:	Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion	:	Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Advice on safe handling	:	Work under hood. Do not inhale substance/mixture.

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Avoid generation of vapours/aerosols.

Further information on storage conditions : Tightly closed.
Keep away from heat and sources of ignition.

Storage class : 4.3, Hazardous materials, which set free flammable gases upon contact with water

Recommended storage temperature : 36 - 46 °F / 2 - 8 °C

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
pentane	109-66-0	C	610 ppm 1,800 mg/m3	NIOSH REL
		TWA	120 ppm 350 mg/m3	NIOSH REL
		TWA	1,000 ppm 2,950 mg/m3	OSHA Z-1
		TWA	1,000 ppm	ACGIH

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type AX

The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Remarks : required

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Eye protection	:	Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles
Skin and body protection	:	Flame retardant antistatic protective clothing.
Hygiene measures	:	Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	:	liquid
Color	:	No data available
Odor	:	No data available
Odor Threshold	:	No data available
pH	:	No data available
Melting point	:	No data available
Boiling point/boiling range	:	95 - 97 °F / 35 - 36 °C
Flash point	:	-31 °F / -35 °C Method: closed cup
Evaporation rate	:	No data available
Flammability (solid, gas)	:	No data available
Flammability (liquids)	:	No data available
Burning rate	:	No data available
Upper explosion limit / Upper flammability limit	:	No data available
Lower explosion limit / Lower flammability limit	:	No data available
Vapor pressure	:	No data available
Relative vapor density	:	No data available

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Relative density	:	No data available
Density	:	0.632 g/mL (77 °F / 25 °C)
Water solubility	:	No data available
Partition coefficient: n-octanol/water	:	No data available
Autoignition temperature	:	No data available
Decomposition temperature	:	No data available
Viscosity, dynamic	:	No data available
Viscosity, kinematic	:	No data available
Flow time	:	No data available
Explosive properties	:	Not classified as explosive.
Oxidizing properties	:	none
Molecular weight	:	50.03 g/mol
Particle characteristics Particle size	:	No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	:	Vapors may form explosive mixture with air.
Chemical stability	:	The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	:	No data available
Conditions to avoid	:	Warming.
Incompatible materials	:	Forms shock-sensitive mixtures with certain other materials. Iron and iron salts. Heavy metals phosphorous Sulfur compounds Oxygen Nickel Do not store near acids.

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Metals
Chlorinated solvents

Hazardous decomposition products : In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Mixture

Acute toxicity
Oral: No data available
Acute toxicity estimate Oral - 2,591 mg/kg
(Calculation method)
Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.
Acute toxicity estimate Inhalation - 4 h - 25.91 mg/l - vapor(Calculation method)

Symptoms: Possible symptoms:, mucosal irritations
Dermal: No data available

Skin corrosion/irritation
Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation
Remarks: Mixture causes serious eye damage.

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

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11.2 Additional Information

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Headache, Nausea, Large doses of lithium ion have caused dizziness and prostration, and can cause kidney damage if sodium intake is limited. Dehydration, weight loss, dermatological effects, and thyroid disturbances have been reported. Central nervous system effects that include slurred speech, blurred vision, sensory loss, ataxia, and convulsions may occur. Diarrhea, vomiting, and neuromuscular effects such as tremor, clonus, and hyperactive reflexes may occur as a result of repeated exposure to lithium ion.
Contact with eyes can cause:, Redness, Blurred vision, Provokes tears., Prolonged or repeated contact with skin may cause:, defatting, Dermatitis, Central nervous system depression, Damage to the lungs.
Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Components

pentane

Acute toxicity
LD50 Oral - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 401)
LC50 Inhalation - Rat - male and female - 4 h - > 25.3 mg/l - vapor
(OECD Test Guideline 403)
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: cyclopentane
Dermal: No data available
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)

Respiratory or skin sensitization
Buehler Test - Guinea pig

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Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity
Test Type: Mutagenicity (mammal cell test): chromosome aberration.
Test system: Chinese hamster ovary cells
Result: negative
Test Type: Ames test
Test system: Salmonella typhimurium
Result: negative
Method: Mutagenicity (micronucleus test)
Species: Rat - male and female - Bone marrow
Result: negative

Carcinogenicity

IARC:	No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
NTP:	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA:	No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
May cause drowsiness or dizziness. - Central nervous system

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
May be fatal if swallowed and enters airways.Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

isopropyllithium

Acute toxicity
Oral: No data available
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

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Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

pentane:

Toxicity to fish	:	LC50 (Oncorhynchus mykiss (rainbow trout)): 4.26 mg/l End point: mortality Exposure time: 96 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 203 GLP: yes
Toxicity to daphnia and other aquatic invertebrates	:	EC50 (Daphnia magna (Water flea)): 2.7 mg/l Exposure time: 48 h Test Type: static test Analytical monitoring: yes Remarks: (ECHA)
Toxicity to algae/aquatic plants	:	ErC50 (Selenastrum capricornutum (green algae)): 10.7 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes NOEC (Selenastrum capricornutum (green algae)): 7.51 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes

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Method: OECD Test Guideline 201
GLP: yes

Ecotoxicology Assessment

Chronic aquatic toxicity : Toxic to aquatic life with long lasting effects.

isopropyllithium:

Toxicity to fish : Remarks: No data available

Persistence and degradability

Components:

pentane:

Biodegradability : aerobic
Inoculum: activated sludge
Concentration: 60 mg/l
Result: Readily biodegradable.
Biodegradation: 87 %
Exposure time: 28 d
Method: OECD Test Guideline 301F
GLP: yes

Bioaccumulative potential

Components:

pentane:

Bioaccumulation : Remarks: No data available

Partition coefficient: n-octanol/water : log Pow: 3.45 (77 °F / 25 °C)
pH: 7
Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Components:

pentane:

Additional ecological information : Avoid release to the environment.
Do not empty into drains.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave

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chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No.	:	UN 3399
Proper shipping name	:	Organometallic substance, liquid, water-reactive, flammable (pentane)
Class	:	4.3
Subsidiary risk	:	3
Packing group	:	I
Labels	:	Division 4.3 - Substances which in contact with water emit flammable gases, Class 3 - Flammable liquids
Packing instruction (cargo aircraft)	:	494
Packing instruction (passenger aircraft)	:	Not permitted for transport

IMDG-Code

UN number	:	UN 3399
Proper shipping name	:	ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE (pentane)
Class	:	4.3
Subsidiary risk	:	3
Packing group	:	I
Labels	:	4.3 (3)
EmS Code	:	F-G, S-N
Marine pollutant	:	yes

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National regulation

49 CFR Road

UN/ID/NA number	:	UN 3399
Proper shipping name	:	Organometallic substance, liquid, water-reactive, flammable (pentane)
Class	:	4.3
Subsidiary risk	:	3
Packing group	:	I
Labels	:	Division 4.3 - Substances which in contact with water emit flammable gases, Class 3 - Flammable liquids
ERG Code	:	138
Marine pollutant	:	no

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Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

Components	CAS-No.	Component TPQ (lbs)

SARA 311/312 Hazards : Fire Hazard
Reactivity Hazard
Acute Health Hazard
Chronic Health Hazard

SARA 313 : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

US State Regulations

Massachusetts Right To Know

pentane 109-66-0

Pennsylvania Right To Know

pentane 109-66-0

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

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No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH	:	USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL	:	USA. NIOSH Recommended Exposure Limits
OSHA Z-1	:	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
ACGIH / TWA	:	8-hour, time-weighted average
NIOSH REL / TWA	:	Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek
NIOSH REL / C	:	Ceiling value not be exceeded at any time.
OSHA Z-1 / TWA	:	8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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US / EN

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