

1. Identification

Product identifier	LIMEDIENE™	
Other means of identification		
BRI Product Code	962	
CAS number	30640-46-1	
FEMA number	4311	
Synonyms	Cyclohexadiene, methyl- * Cyclohexadiene, methyl- (Mixture of isomers) * Lemon hexadiene * Methyl Cyclohexadiene * Mixture of methyl cyclohexadiene and methylene cyclohexene	
Recommended use	flavors and fragrances For Manufacturing Use Only	
Recommended restrictions	Not for use in Tobacco or Nicotine delivery device applications and/or products.	
Manufacturer/Importer/Supplier/Distributor information		
Manufacturer		
Company name	Bedoukian Research Inc (BRI)	
Address	6 Commerce Drive Danbury, CT 06810 United States	
Telephone	1-203-830-4000	
Website	www.bedoukian.com	
E-mail	customerservice@bedoukian.com	
Contact person	Joseph Bania	
Emergency phone number	Chemtrec (North America)	1-800-424-9300
	Chemtrec (International)	+1-703-527-3887

2. Hazard(s) identification

Physical hazards	Flammable liquids	Category 2
Health hazards	Aspiration hazard	Category 1
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	

Label elements



Signal word	Danger
Hazard statement	Highly flammable liquid and vapor. May be fatal if swallowed and enters airways.
Precautionary statement	
Prevention	Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Keep container tightly closed. Ground/bond container and receiving equipment. Use explosion-proof electrical/ventilating/lighting equipment. Use only non-sparking tools. Take precautionary measures against static discharge. Wear protective gloves/eye protection/face protection.
Response	If swallowed: Immediately call a poison center/doctor. Do NOT induce vomiting. If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower. In case of fire: Use appropriate media to extinguish.
Storage	Store in a well-ventilated place. Keep cool. Store locked up.
Disposal	Dispose of contents/container in accordance with relevant area regulations.
Hazard(s) not otherwise classified (HNOC)	None known.
Supplemental information	Contains synthetic alpha tocopherol. May produce an allergic reaction.

3. Composition/information on ingredients

Substances

Chemical name	Common name and synonyms	CAS number	%
LIMEDIENE™	Cyclohexadiene, methyl- Cyclohexadiene, methyl- (Mixture of isomers) Lemon hexadiene Methyl Cyclohexadiene Mixture of methyl cyclohexadiene and methylene cyclohexene	30640-46-1	99.2

Impurities

Chemical name	Common name and synonyms	CAS number	%
Toluene		108-88-3	< 0.3

Stabilizers

Chemical name	Common name and synonyms	CAS number	%
synthetic alpha tocopherol		10191-41-0	0.5

*Designates that a specific chemical identity and/or percentage of composition has been withheld as a trade secret.

Composition comments Occupational Exposure Limits for impurities are listed in Section 8. Occupational Exposure Limits for stabilizers are listed in Section 8.

4. First-aid measures

Inhalation

Move to fresh air. Call a physician if symptoms develop or persist.

Skin contact

Take off immediately all contaminated clothing. Rinse skin with water/shower. Get medical attention if irritation develops and persists.

Eye contact

Immediately flush eyes with plenty of water for at least 15 minutes. Remove contact lenses, if present and easy to do. Get medical attention if irritation develops and persists.

Ingestion

Call a physician or poison control center immediately. Rinse mouth. Do not induce vomiting. If vomiting occurs, keep head low so that stomach content doesn't get into the lungs.

Most important symptoms/effects, acute and delayed

Aspiration may cause pulmonary edema and pneumonitis. Direct contact with eyes may cause temporary irritation.

Indication of immediate medical attention and special treatment needed

Provide general supportive measures and treat symptomatically. Thermal burns: Flush with water immediately. While flushing, remove clothes which do not adhere to affected area. Call an ambulance. Continue flushing during transport to hospital. Keep victim under observation. Symptoms may be delayed.

General information

Take off all contaminated clothing immediately. Ensure that medical personnel are aware of the material(s) involved, and take precautions to protect themselves. Wash contaminated clothing before reuse.

5. Fire-fighting measures

Suitable extinguishing media

Water fog. Foam. Dry chemical powder. Carbon dioxide (CO₂).

Unsuitable extinguishing media

Do not use water jet as an extinguisher, as this will spread the fire.

Specific hazards arising from the chemical

Vapors may form explosive mixtures with air. Vapors may travel considerable distance to a source of ignition and flash back. During fire, gases hazardous to health may be formed.

Special protective equipment and precautions for firefighters

Self-contained breathing apparatus and full protective clothing must be worn in case of fire.

Fire fighting equipment/instructions

In case of fire and/or explosion do not breathe fumes. Move containers from fire area if you can do so without risk.

Specific methods

Use standard firefighting procedures and consider the hazards of other involved materials.

General fire hazards

Highly flammable liquid and vapor.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Keep unnecessary personnel away. Keep people away from and upwind of spill/leak. Eliminate all ignition sources (no smoking, flares, sparks, or flames in immediate area). Wear appropriate protective equipment and clothing during clean-up. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Ventilate closed spaces before entering them. Local authorities should be advised if significant spillages cannot be contained. For personal protection, see section 8 of the SDS.

Methods and materials for containment and cleaning up

Eliminate all ignition sources (no smoking, flares, sparks, or flames in immediate area). Keep combustibles (wood, paper, oil, etc.) away from spilled material. Take precautionary measures against static discharge. Use only non-sparking tools.

Large Spills: Stop the flow of material, if this is without risk. Dike the spilled material, where this is possible. Use a non-combustible material like vermiculite, sand or earth to soak up the product and place into a container for later disposal. Following product recovery, flush area with water.

Small Spills: Absorb with earth, sand or other non-combustible material and transfer to containers for later disposal. Clean surface thoroughly to remove residual contamination.

Never return spills to original containers for re-use. For waste disposal, see section 13 of the SDS. Avoid discharge into drains, water courses or onto the ground.

Environmental precautions

7. Handling and storage

Precautions for safe handling

Do not handle, store or open near an open flame, sources of heat or sources of ignition. Protect material from direct sunlight. When using do not smoke. Explosion-proof general and local exhaust ventilation. Take precautionary measures against static discharges. All equipment used when handling the product must be grounded. Use non-sparking tools and explosion-proof equipment. Wear appropriate personal protective equipment. Wash hands thoroughly after handling. Observe good industrial hygiene practices.

Conditions for safe storage, including any incompatibilities

Store locked up. Keep away from heat, sparks and open flame. Prevent electrostatic charge build-up by using common bonding and grounding techniques. Store in a cool, dry place out of direct sunlight. Store in original tightly closed container. Store in a well-ventilated place. Keep in an area equipped with sprinklers. Store away from incompatible materials (see Section 10 of the SDS). Recommended Packaging: Glass, Aluminum or Phenolic Lined Steel. Store tightly sealed under inert gas below 0 deg. C

8. Exposure controls/personal protection

Occupational exposure limits

US. OSHA Table Z-2 (29 CFR 1910.1000)

Impurities	Type	Value
Toluene (CAS 108-88-3)	Ceiling	300 ppm
	TWA	200 ppm

US. ACGIH Threshold Limit Values

Impurities	Type	Value
Toluene (CAS 108-88-3)	TWA	20 ppm

US. NIOSH: Pocket Guide to Chemical Hazards

Impurities	Type	Value
Toluene (CAS 108-88-3)	STEL	560 mg/m ³
	TWA	150 ppm
		375 mg/m ³
		100 ppm

Biological limit values

ACGIH Biological Exposure Indices

Impurities	Value	Determinant	Specimen	Sampling Time
Toluene (CAS 108-88-3)	0.3 mg/g	o-Cresol, with hydrolysis	Creatinine in urine	*
	0.03 mg/l	Toluene	Urine	*
	0.02 mg/l	Toluene	Blood	*

* - For sampling details, please see the source document.

Exposure guidelines

US - California OELs: Skin designation

Toluene (CAS 108-88-3) Can be absorbed through the skin.

US - Minnesota Haz Subs: Skin designation applies

Toluene (CAS 108-88-3) Skin designation applies.

Appropriate engineering controls	Explosion-proof general and local exhaust ventilation. Eye wash fountain and emergency showers are recommended.
Individual protection measures, such as personal protective equipment	
Eye/face protection	Face shield is recommended. Wear safety glasses with side shields (or goggles).
Skin protection	
Hand protection	Wear appropriate chemical resistant gloves.
Other	Wear suitable protective clothing.
Respiratory protection	If engineering controls do not maintain airborne concentrations below recommended exposure limits (where applicable) or to an acceptable level (in countries where exposure limits have not been established), an approved respirator must be worn.
Thermal hazards	Wear appropriate thermal protective clothing, when necessary.
General hygiene considerations	When using do not smoke. Always observe good personal hygiene measures, such as washing after handling the material and before eating, drinking, and/or smoking. Routinely wash work clothing and protective equipment to remove contaminants.

9. Physical and chemical properties

Appearance

Physical state	Liquid.
Color	colorless to yellow
Odor	powerful lemon-lime top note.
Odor threshold	Not available.
pH	Not available.
Melting point/freezing point	Not available.
Initial boiling point and boiling range	244.08 °F (117.82 °C) US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Flash point	35 °F (2 °C) Closed Cup
Evaporation rate	Not available.
Flammability (solid, gas)	Not applicable.
Upper/lower flammability or explosive limits	
Flammability limit - lower (%)	Not available.
Flammability limit - upper (%)	Not available.
Explosive limit - lower (%)	Not available.
Explosive limit - upper (%)	Not available.
Vapor pressure	15.6 mmHg at 20°C; US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Vapor density	3.2 Relative to air; air = 1
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Not available.
Partition coefficient (n-octanol/water)	3.29 US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Auto-ignition temperature	Not available.
Decomposition temperature	Not available.
Viscosity	Not available.
Other information	
Density	0.830 - 0.837 g/cm ³
Dynamic viscosity	0.92 cP at 10.3°C. Bedoukian obtained value.
Explosive properties	Not explosive.
Flammability class	Flammable IB estimated
Molecular formula	C ₇ H ₁₀
Molecular weight	94.15

Oxidizing properties Not oxidizing.
Specific gravity 0.83 - 0.837 at 25°C

10. Stability and reactivity

Reactivity The product is stable and non-reactive under normal conditions of use, storage and transport.
Chemical stability Material is stable under normal conditions.
Possibility of hazardous reactions Hazardous polymerization does not occur.
Conditions to avoid Avoid heat, sparks, open flames and other ignition sources. Avoid temperatures exceeding the flash point. Contact with incompatible materials.
Incompatible materials Strong oxidizing agents.
Hazardous decomposition products No hazardous decomposition products are known.

11. Toxicological information

Information on likely routes of exposure

Inhalation May cause allergy or asthma symptoms or breathing difficulties if inhaled.
Skin contact May cause an allergic skin reaction.
Eye contact Direct contact with eyes may cause temporary irritation.
Ingestion Droplets of the product aspirated into the lungs through ingestion or vomiting may cause a serious chemical pneumonia.
Symptoms related to the physical, chemical and toxicological characteristics Aspiration may cause pulmonary edema and pneumonitis.

Information on toxicological effects

Acute toxicity May be fatal if swallowed and enters airways.

Product	Species	Test Results
LIMEDIENE™ (CAS 30640-46-1)		
Acute		
Inhalation		
<i>Mist</i>		
LC50	Rat	> 5.16 mg/l
Oral		
<i>Liquid</i>		
LD50	Rat	> 2000 mg/kg

* Estimates for product may be based on additional component data not shown.

Skin corrosion/irritation Prolonged skin contact may cause temporary irritation.

Irritation Corrosion - Skin LIMEDIENE™

100 % Buehler, Preliminary irritation study as part of a skin sensitization assay.
Result: Not irritating.
Species: Guinea pig
Organ: Skin
Notes: BRI study

Serious eye damage/eye irritation Direct contact with eyes may cause temporary irritation.

Respiratory or skin sensitization

Respiratory sensitization Not a respiratory sensitizer.

Skin sensitization This product is not expected to cause skin sensitization.

Skin sensitization LIMEDIENE™

100 % Buehler
Result: Not sensitizing.
Species: Guinea pig
Organ: Skin
Notes: BRI study

Germ cell mutagenicity No data available to indicate product or any components present at greater than 0.1% are mutagenic or genotoxic.

Germ cell mutagenicity: Ames test
LIMEDIENE™

OECD 471, Strain WP2 trp uvrA with and without metabolic activation. Vehicle Acetone.
Result: Not mutagenic.
Species: Escherichia coli
OECD 471, Strains TA 97a, TA 98, TA 100, and TA 1535 with and without metabolic activation. Vehicle Acetone.
Result: Not mutagenic.
Species: Salmonella typhimurium

Carcinogenicity Not classifiable as to carcinogenicity to humans.

IARC Monographs. Overall Evaluation of Carcinogenicity

Toluene (CAS 108-88-3)

3 Not classifiable as to carcinogenicity to humans.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)

Not regulated.

US. National Toxicology Program (NTP) Report on Carcinogens

Not listed.

Reproductive toxicity This product is not expected to cause reproductive or developmental effects.

Specific target organ toxicity - single exposure Not classified.

Specific target organ toxicity - repeated exposure Not classified.

Aspiration hazard May be fatal if swallowed and enters airways.

Further information May cause allergic respiratory and skin reactions.

12. Ecological information

Ecotoxicity The product is not classified as environmentally hazardous. However, this does not exclude the possibility that large or frequent spills can have a harmful or damaging effect on the environment.

Impurities	Species	Test Results	
Toluene (CAS 108-88-3)			
Aquatic			
Crustacea	EC50	Water flea (Daphnia magna)	5.46 - 9.83 mg/l, 48 hours
Fish	LC50	Coho salmon, silver salmon (Oncorhynchus kisutch)	8.11 mg/l, 96 hours

* Estimates for product may be based on additional component data not shown.

Persistence and degradability The product is readily biodegradable.

Biodegradability

Percent degradation (Aerobic biodegradation-ready)

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OECD 301F, 100 mg/L. 69% biodegradation after 28 days (72% after 36 days) in the test conditions. Under the conditions of the study, the test material should be regarded as readily biodegradable.
Result: Readily biodegradable.
Species: Activated sludge of a predominantly domestic sewage

Bioaccumulative potential

Partition coefficient n-octanol / water (log Kow)

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3.29, US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.

Mobility in soil No data available.

Other adverse effects No other adverse environmental effects (e.g. ozone depletion, photochemical ozone creation potential, endocrine disruption, global warming potential) are expected from this component.

13. Disposal considerations

Disposal instructions Collect and reclaim or dispose in sealed containers at licensed waste disposal site. Dispose of contents/container in accordance with local/regional/national/international regulations.

Local disposal regulations	Dispose in accordance with all applicable regulations.
Hazardous waste code	The waste code should be assigned in discussion between the user, the producer and the waste disposal company.
Waste from residues / unused products	Dispose of in accordance with local regulations. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe manner (see: Disposal instructions).
Contaminated packaging	Since emptied containers may retain product residue, follow label warnings even after container is emptied. Empty containers should be taken to an approved waste handling site for recycling or disposal.

14. Transport information

DOT

UN number	UN1993
UN proper shipping name	Flammable liquids, n.o.s. (Methyl Cyclohexadiene)
Transport hazard class(es)	
Class	3
Subsidiary risk	-
Label(s)	3
Packing group	II
Special precautions for user	Read safety instructions, SDS and emergency procedures before handling.
Special provisions	IB2, T7, TP1, TP8, TP28
Packaging exceptions	150
Packaging non bulk	202
Packaging bulk	242

IATA

UN number	UN1993
UN proper shipping name	Flammable liquid, n.o.s. (Methyl Cyclohexadiene)
Transport hazard class(es)	
Class	3
Subsidiary risk	-
Packing group	II
Environmental hazards	No.
ERG Code	3H
Special precautions for user	Read safety instructions, SDS and emergency procedures before handling.
Other information	
Passenger and cargo aircraft	Allowed with restrictions.
Cargo aircraft only	Allowed with restrictions.

IMDG

UN number	UN1993
UN proper shipping name	FLAMMABLE LIQUID, N.O.S. (Methyl Cyclohexadiene)
Transport hazard class(es)	
Class	3
Subsidiary risk	-
Packing group	II
Environmental hazards	
Marine pollutant	No.
EmS	F-E, S-E
Special precautions for user	Read safety instructions, SDS and emergency procedures before handling.
Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	Not established.

DOT



IATA; IMDG



15. Regulatory information

US federal regulations

This product is a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.

TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)

Not regulated.

CERCLA Hazardous Substance List (40 CFR 302.4)

Toluene (CAS 108-88-3)

Listed.

SARA 304 Emergency release notification

Not regulated.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)

Not regulated.

Superfund Amendments and Reauthorization Act of 1986 (SARA)

Hazard categories

Immediate Hazard - Yes
Delayed Hazard - No
Fire Hazard - Yes
Pressure Hazard - No
Reactivity Hazard - No

SARA 302 Extremely hazardous substance

Not listed.

SARA 311/312 Hazardous chemical

Yes

SARA 313 (TRI reporting)

Not regulated.

Other federal regulations

Clean Air Act (CAA) Section 112 Hazardous Air Pollutants (HAPs) List

Toluene (CAS 108-88-3)

Clean Air Act (CAA) Section 112(r) Accidental Release Prevention (40 CFR 68.130)

Not regulated.

Safe Drinking Water Act (SDWA)

Not regulated.

US state regulations

WARNING: This product contains a chemical known to the State of California to cause birth defects or other reproductive harm.

US - California Proposition 65 - CRT: Listed date/Developmental toxin

Toluene (CAS 108-88-3)

Listed: January 1, 1991

US. California. Candidate Chemicals List. Safer Consumer Products Regulations (Cal. Code Regs, tit. 22, 69502.3, subd. (a))

Toluene (CAS 108-88-3)

International Inventories

Country(s) or region	Inventory name	On inventory (yes/no)*
Australia	Australian Inventory of Chemical Substances (AICS)	Yes
Canada	Domestic Substances List (DSL)	Yes
Canada	Non-Domestic Substances List (NDSL)	No
China	Inventory of Existing Chemical Substances in China (IECSC)	Yes
Europe	European Inventory of Existing Commercial Chemical Substances (EINECS)	Yes
Europe	European List of Notified Chemical Substances (ELINCS)	No
Japan	Inventory of Existing and New Chemical Substances (ENCS)	No
Korea	Existing Chemicals List (ECL)	No
New Zealand	New Zealand Inventory	Yes
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	No
Taiwan	Taiwan Toxic Chemical Substances (TCS)	Yes
United States & Puerto Rico	Toxic Substances Control Act (TSCA) Inventory	Yes

*A "Yes" indicates that all components of this product comply with the inventory requirements administered by the governing country(s)

A "No" indicates that one or more components of the product are not listed or exempt from listing on the inventory administered by the governing country(s).

16. Other information, including date of preparation or last revision

Issue date 13-October-2021

Revision date 29-February-2024

Version # 06

Disclaimer Bedoukian Research Inc (BRI) cannot anticipate all conditions under which this information and its product, or the products of other manufacturers in combination with its product, may be used. It is the user's responsibility to ensure safe conditions for handling, storage and disposal of the product, and to assume liability for loss, injury, damage or expense due to improper use. The information in the sheet was written based on the best knowledge and experience currently available.

Revision information Hazard(s) identification: Disposal
Hazard(s) identification: Supplemental information
Composition / Information on Ingredients: Disclosure Overrides
Physical & Chemical Properties: Multiple Properties
Physical and chemical properties: Color
Toxicological Information: Toxicological Property Data
Toxicological information: Further information
Toxicological information: Inhalation
Toxicological information: Skin contact