

1. Identification

Product identifier	4-PENTENOIC ACID
Other means of identification	
BRI Product Code	448
CAS number	591-80-0
FEMA number	2843
Synonyms	4-Pentenoic acid * Allyl acetic acid * Allylacetic acid
Recommended use	flavors only 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	
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 4
Health hazards	Acute toxicity, oral	Category 4
	Skin corrosion/irritation	Category 1
	Serious eye damage/eye irritation	Category 1
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	
Label elements		



Signal word	Danger
Hazard statement	Combustible liquid. Harmful if swallowed. Causes severe skin burns and eye damage. Causes serious eye damage.
Precautionary statement	
Prevention	Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Do not breathe mist or vapor. Wash thoroughly after handling. Do not eat, drink or smoke when using this product. Wear protective gloves/protective clothing/eye protection/face protection.
Response	If swallowed: Rinse mouth. Do NOT induce vomiting. If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower. If inhaled: Remove person to fresh air and keep comfortable for breathing. 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. Wash contaminated clothing before reuse. 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 None.

3. Composition/information on ingredients

Substances

Chemical name	Common name and synonyms	CAS number	%
4-PENTENOIC ACID	4-Pentenoic acid Allyl acetic acid Allylacetic acid	591-80-0	100

Stabilizers

Chemical name	Common name and synonyms	CAS number	%
synthetic alpha tocopherol		10191-41-0	0.1

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

Composition comments 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. Call a physician or poison control center immediately. Chemical burns must be treated by a physician. Wash contaminated clothing before reuse.

Eye contact

Immediately flush eyes with plenty of water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Call a physician or poison control center immediately.

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

Burning pain and severe corrosive skin damage. Causes serious eye damage. Symptoms may include stinging, tearing, redness, swelling, and blurred vision. Permanent eye damage including blindness could result.

Indication of immediate medical attention and special treatment needed

Provide general supportive measures and treat symptomatically. Chemical 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 warm. Keep victim under observation. Symptoms may be delayed.

General information

Ensure that medical personnel are aware of the material(s) involved, and take precautions to protect themselves. Show this safety data sheet to the doctor in attendance.

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

The product is combustible, and heating may generate vapors which may form explosive vapor/air mixtures. 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

Combustible liquid.

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 breathe mist or vapor. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Ensure adequate ventilation. 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.

Large Spills: Stop the flow of material, if this is without risk. Dike the spilled material, where this is possible. Cover with plastic sheet to prevent spreading. 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. Wipe up with absorbent material (e.g. cloth, fleece). 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

Keep away from open flames, hot surfaces and sources of ignition. Do not breathe mist or vapor. Do not get in eyes, on skin, or on clothing. Do not taste or swallow. When using, do not eat, drink or smoke. Provide adequate ventilation. 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. 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 or Plastic. Store tightly sealed under inert gas in a cool, well-ventilated area.

8. Exposure controls/personal protection

Occupational exposure limits

This substance has no PEL, TLV, or other recommended exposure limit.

Biological limit values

No biological exposure limits noted for the ingredient(s).

Appropriate engineering controls

Good general ventilation (typically 10 air changes per hour) should be used. Ventilation rates should be matched to conditions. If applicable, use process enclosures, local exhaust ventilation, or other engineering controls to maintain airborne levels below recommended exposure limits. If exposure limits have not been established, maintain airborne levels to an acceptable level. Eye wash facilities and emergency shower must be available when handling this product.

Individual protection measures, such as personal protective equipment

Eye/face protection

Wear safety glasses with side shields (or goggles) and a face shield.

Skin protection

Hand protection

Wear appropriate chemical resistant gloves. Suitable gloves can be recommended by the glove supplier.

Other

Wear appropriate chemical resistant 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. Keep away from food and drink. 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 pale yellow

Odor

cheese-like aroma.

Odor threshold

Not available.

pH

Not available.

Melting point/freezing point

Not available.

Initial boiling point and boiling range

371.3 °F (188.5 °C) Literature reference.

Flash point

188 °F (87 °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	0.44 mmHg at 20°C; US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Vapor density	3.5 Relative to air; air = 1
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Not available.
Partition coefficient (n-octanol/water)	1.42 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	0.971 - 0.979 g/cm3
Flammability class	Combustible IIIA estimated
Molecular formula	C5H8O2
Molecular weight	100.11
Specific gravity	0.971 - 0.979 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 irritation to the respiratory system.
Skin contact	Causes severe skin burns.
Eye contact	Causes serious eye damage.
Ingestion	Causes digestive tract burns. Harmful if swallowed.
Symptoms related to the physical, chemical and toxicological characteristics	Burning pain and severe corrosive skin damage. Causes serious eye damage. Symptoms may include stinging, tearing, redness, swelling, and blurred vision. Permanent eye damage including blindness could result.
Information on toxicological effects	
Acute toxicity	Harmful if swallowed.

Product	Species	Test Results
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4-PENTENOIC ACID (CAS 591-80-0)

Acute

Oral

Liquid

LD50

Rat

470 mg/kg

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

Skin corrosion/irritation

Causes severe skin burns and eye damage.

Serious eye damage/eye irritation

Causes serious eye damage.

Respiratory or skin sensitization

Respiratory sensitization

Not a respiratory sensitizer.

Skin sensitization

This product is not expected to cause skin sensitization.

Germ cell mutagenicity

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

Carcinogenicity

This product is not considered to be a carcinogen by IARC, ACGIH, NTP, or OSHA.

IARC Monographs. Overall Evaluation of Carcinogenicity

Not listed.

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

Not an aspiration hazard.

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.

Persistence and degradability

No data is available on the degradability of this product.

Bioaccumulative potential

Partition coefficient n-octanol / water (log Kow)

4-PENTENOIC ACID

1.42, 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	UN2922
UN proper shipping name	Corrosive liquids, toxic, n.o.s. (4-PENTENOIC ACID)
Transport hazard class(es)	
Class	8
Subsidiary risk	6.1(PGIII)
Label(s)	8, 6.1
Packing group	III
Special precautions for user	Read safety instructions, SDS and emergency procedures before handling.
Special provisions	IB3, T7, TP1, TP28
Packaging exceptions	154
Packaging non bulk	203
Packaging bulk	241

IATA

UN number	UN2922
UN proper shipping name	Corrosive liquids, toxic, n.o.s. (4-PENTENOIC ACID)
Transport hazard class(es)	
Class	8
Subsidiary risk	6.1(PGIII)
Packing group	III
Environmental hazards	No.
ERG Code	8P
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	UN2922
UN proper shipping name	CORROSIVE LIQUIDS, TOXIC, N.O.S. (4-PENTENOIC ACID)
Transport hazard class(es)	
Class	8
Subsidiary risk	6.1(PGIII)
Packing group	III
Environmental hazards	
Marine pollutant	No.
EmS	F-A, S-B
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)

Not 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

Not regulated.

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

Not regulated.

Safe Drinking Water Act (SDWA) Not regulated.

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)	Yes
Korea	Existing Chemicals List (ECL)	Yes
New Zealand	New Zealand Inventory	Yes
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	Yes
Taiwan	Taiwan Toxic Chemical Substances (TCS)	Yes

Country(s) or region	Inventory name	On inventory (yes/no)*
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).

IFRA restriction There is an IFRA guideline regarding this product. Please visit www.ifraorg.org for the full text of the guideline, or contact Bedoukian Research, Inc. for more information.

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

Issue date 26-May-2015

Revision date 08-June-2020

Version # 03

Disclaimer Bedoukian Research 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
Physical and chemical properties: Color