

# SAFETY DATA SHEET

## 1. Identification

<b>Product identifier</b>	<b>NUEZATE</b>	
<b>Other means of identification</b>		
<b>BRI Product Code</b>	728	
<b>CAS number</b>	26516-27-8	
<b>FEMA number</b>	4903	
<b>Synonyms</b>	3-Methyl-2-oxo-ethyl-pentanoate * Ethyl 3-methyl-2-oxo-pentanoate * Pentanoic acid, 3-methyl-2-oxo-, ethyl ester	
<b>Recommended use</b>	flavors and fragrances For Manufacturing Use Only	
<b>Recommended restrictions</b>	Not for use in Tobacco or Nicotine delivery device applications and/or products.	
<b>Manufacturer/Importer/Supplier/Distributor information</b>		
<b>Manufacturer</b>		
<b>Company name</b>	Bedoukian Research	
<b>Address</b>	6 Commerce Drive Danbury, CT 06810 United States	
<b>Telephone</b>	1-203-830-4000	
<b>Website</b>	www.bedoukian.com	
<b>E-mail</b>	customerservice@bedoukian.com	
<b>Contact person</b>	Joseph Bania	
<b>Emergency phone number</b>	Chemtrec (North America)	1-800-424-9300
	Chemtrec (International)	1-703-527-3887

## 2. Hazard(s) identification

<b>Physical hazards</b>	Flammable liquids	Category 4
<b>Health hazards</b>	Sensitization, skin	Category 1
<b>Environmental hazards</b>	Not classified.	
<b>OSHA defined hazards</b>	Not classified.	

### Label elements



<b>Signal word</b>	Warning
<b>Hazard statement</b>	Combustible liquid. May cause an allergic skin reaction.
<b>Precautionary statement</b>	
<b>Prevention</b>	Keep away from flames and hot surfaces-No smoking. Avoid breathing mist or vapor. Contaminated work clothing must not be allowed out of the workplace. Wear protective gloves/eye protection/face protection.
<b>Response</b>	If on skin: Wash with plenty of water. If skin irritation or rash occurs: Get medical advice/attention. Wash contaminated clothing before reuse. In case of fire: Use appropriate media to extinguish.
<b>Storage</b>	Store in a well-ventilated place. Keep cool.
<b>Disposal</b>	Dispose of contents/container in accordance with relevant area regulations.
<b>Hazard(s) not otherwise classified (HNOC)</b>	None known.
<b>Supplemental information</b>	100% of the mixture consists of component(s) of unknown acute dermal toxicity. 100% of the mixture consists of component(s) of unknown acute inhalation toxicity. Contains NUEZATE. May produce an allergic reaction.

### 3. Composition/information on ingredients

#### Substances

Chemical name	Common name and synonyms	CAS number	%
NUEZATE	3-Methyl-2-oxo-ethyl-pentanoate Ethyl 3-methyl-2-oxo-pentanoate Pentanoic acid, 3-methyl-2-oxo-, ethyl ester	26516-27-8	100

#### Impurities

Chemical name	Common name and synonyms	CAS number	%
2-BUTANONE		78-93-3	< 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.

### 4. First-aid measures

<b>Inhalation</b>	Move to fresh air. Call a physician if symptoms develop or persist.
<b>Skin contact</b>	Remove contaminated clothing immediately and wash skin with soap and water. In case of eczema or other skin disorders: Seek medical attention and take along these instructions.
<b>Eye contact</b>	Rinse with water. Get medical attention if irritation develops and persists.
<b>Ingestion</b>	Rinse mouth. Get medical attention if symptoms occur.
<b>Most important symptoms/effects, acute and delayed</b>	Direct contact with eyes may cause temporary irritation. May cause an allergic skin reaction. Dermatitis. Rash.
<b>Indication of immediate medical attention and special treatment needed</b>	Provide general supportive measures and treat symptomatically. Keep victim under observation. Symptoms may be delayed.
<b>General information</b>	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

<b>Suitable extinguishing media</b>	Water fog. Foam. Dry chemical powder. Carbon dioxide (CO <sub>2</sub> ).
<b>Unsuitable extinguishing media</b>	Do not use water jet as an extinguisher, as this will spread the fire.
<b>Specific hazards arising from the chemical</b>	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.
<b>Special protective equipment and precautions for firefighters</b>	Self-contained breathing apparatus and full protective clothing must be worn in case of fire.
<b>Fire fighting equipment/instructions</b>	In case of fire and/or explosion do not breathe fumes. Move containers from fire area if you can do so without risk.
<b>Specific methods</b>	Use standard firefighting procedures and consider the hazards of other involved materials.
<b>General fire hazards</b>	Combustible liquid.

### 6. Accidental release measures

<b>Personal precautions, protective equipment and emergency procedures</b>	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. Avoid breathing 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.
<b>Methods and materials for containment and cleaning up</b>	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. 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.

**Environmental precautions** Avoid discharge into drains, water courses or onto the ground.

## 7. Handling and storage

**Precautions for safe handling** Keep away from open flames, hot surfaces and sources of ignition. When using do not smoke. Avoid breathing mist or vapor. Avoid contact with eyes, skin, and clothing. Provide adequate ventilation. Wear appropriate personal protective equipment. Observe good industrial hygiene practices.

**Conditions for safe storage, including any incompatibilities** 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, Plastic, Aluminum or Phenolic Lined Steel. Store tightly sealed under inert gas in a cool, well-ventilated area.

## 8. Exposure controls/personal protection

### Occupational exposure limits

#### US. OSHA Table Z-1 Limits for Air Contaminants (29 CFR 1910.1000)

Impurities	Type	Value
2-BUTANONE (CAS 78-93-3)	PEL	590 mg/m3
		200 ppm

#### US. ACGIH Threshold Limit Values

Impurities	Type	Value
2-BUTANONE (CAS 78-93-3)	STEL	300 ppm
	TWA	200 ppm

#### US. NIOSH: Pocket Guide to Chemical Hazards

Impurities	Type	Value
2-BUTANONE (CAS 78-93-3)	STEL	885 mg/m3
		300 ppm
	TWA	590 mg/m3 200 ppm

### Biological limit values

#### ACGIH Biological Exposure Indices

Impurities	Value	Determinant	Specimen	Sampling Time
2-BUTANONE (CAS 78-93-3)	2 mg/l	MEK	Urine	*

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

**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.

### 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 appropriate chemical resistant clothing. Use of an impervious apron is recommended.

**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. Contaminated work clothing should not be allowed out of the workplace.

## 9. Physical and chemical properties

### Appearance

Material name: NUEZATE

728 Version #: 05 Revision date: 17-November-2020 Issue date: 27-March-2018

SDS US

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<b>Physical state</b>	Liquid.
<b>Color</b>	pale yellow to yellow
<b>Odor</b>	sweet, walnut, slightly earthy
<b>Odor threshold</b>	Not available.
<b>pH</b>	Not available.
<b>Melting point/freezing point</b>	Not available.
<b>Initial boiling point and boiling range</b>	388.22 °F (197.9 °C) US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
<b>Flash point</b>	157 °F (69 °C) Closed Cup Bedoukian obtained value.
<b>Evaporation rate</b>	Not available.
<b>Flammability (solid, gas)</b>	Not applicable.
<b>Upper/lower flammability or explosive limits</b>	
<b>Flammability limit - lower (%)</b>	Not available.
<b>Flammability limit - upper (%)</b>	Not available.
<b>Explosive limit - lower (%)</b>	Not available.
<b>Explosive limit - upper (%)</b>	Not available.
<b>Vapor pressure</b>	0.27 mmHg at 20°C; US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
<b>Vapor density</b>	5.5 Relative to air; air = 1
<b>Relative density</b>	Not available.
<b>Solubility(ies)</b>	
<b>Solubility (water)</b>	Not available.
<b>Partition coefficient (n-octanol/water)</b>	0.934 US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
<b>Auto-ignition temperature</b>	Not available.
<b>Decomposition temperature</b>	Not available.
<b>Viscosity</b>	Not available.
<b>Other information</b>	
<b>Density</b>	0.963 - 0.969 g/cm <sup>3</sup>
<b>Explosive properties</b>	Not explosive.
<b>Flammability class</b>	Combustible IIIA estimated
<b>Molecular formula</b>	C <sub>8</sub> H <sub>14</sub> O <sub>3</sub>
<b>Molecular weight</b>	158.20
<b>Oxidizing properties</b>	Not oxidizing.
<b>Specific gravity</b>	0.963 - 0.969 at 25°C

## 10. Stability and reactivity

<b>Reactivity</b>	The product is stable and non-reactive under normal conditions of use, storage and transport.
<b>Chemical stability</b>	Material is stable under normal conditions.
<b>Possibility of hazardous reactions</b>	No dangerous reaction known under conditions of normal use.
<b>Conditions to avoid</b>	Avoid heat, sparks, open flames and other ignition sources. Avoid temperatures exceeding the flash point. Contact with incompatible materials.
<b>Incompatible materials</b>	Strong oxidizing agents.
<b>Hazardous decomposition products</b>	No hazardous decomposition products are known.

## 11. Toxicological information

### Information on likely routes of exposure

<b>Inhalation</b>	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
<b>Skin contact</b>	May cause an allergic skin reaction.

**Eye contact** Direct contact with eyes may cause temporary irritation.

**Ingestion** Expected to be a low ingestion hazard.

**Symptoms related to the physical, chemical and toxicological characteristics** May cause an allergic skin reaction. Dermatitis. Rash.

**Information on toxicological effects**

**Acute toxicity** Not known.

Product	Species	Test Results
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NUEZATE (CAS 26516-27-8)

**Acute**

**Oral**

*Liquid*

LD50

Rat

> 2000 mg/kg

Impurities	Species	Test Results
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2-BUTANONE (CAS 78-93-3)

**Acute**

**Oral**

LD50

Rat

2300 - 3500 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**  
NUEZATE

100 % OECD 404  
Result: Not irritating.  
Species: Rabbit  
Organ: Skin

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

**Irritation Corrosion - Eye**  
NUEZATE

OECD 405, Data from literature, details unknown.  
Result: Not irritating.  
Species: Rabbit  
Organ: Eye  
Notes: Firmenich SDS

**Respiratory or skin sensitization**

**Respiratory sensitization** Not a respiratory sensitizer.

**Skin sensitization** May cause an allergic skin reaction.

**Skin sensitization**  
NUEZATE

OECD 406, Data from literature, details unknown.  
Result: Sensitization noted.  
Species: Guinea pig  
Organ: skin  
Notes: Firmenich SDS

**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**  
NUEZATE

OECD 471, Data from literature, details unknown.  
Result: Not mutagenic.  
Species: Salmonella typhimurium  
Notes: Firmenich SDS

**Carcinogenicity** Not classifiable as to carcinogenicity to humans.

**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.

<b>Reproductive toxicity</b>	This product is not expected to cause reproductive or developmental effects.
<b>Specific target organ toxicity - single exposure</b>	Not classified.
<b>Specific target organ toxicity - repeated exposure</b>	Not classified.
<b>Aspiration hazard</b>	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.

Impurities	Species		Test Results
2-BUTANONE (CAS 78-93-3)			
<b>Aquatic</b>			
Crustacea	EC50	Water flea ( <i>Daphnia magna</i> )	4025 - 6440 mg/l, 48 hours
Fish	LC50	Sheepshead minnow ( <i>Cyprinodon variegatus</i> )	> 400 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)

NUEZATE

OECD 301D, 10-day criteria fulfilled.  
Result: Readily biodegradable.  
Species: activated sludge (adaptation not specified)

### Bioaccumulative potential

#### Partition coefficient n-octanol / water (log Kow)

NUEZATE

0.934, 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.

#### US RCRA Hazardous Waste U List: Reference

2-BUTANONE (CAS 78-93-3)

U159

### 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

Not regulated as dangerous goods.

### IATA

Not regulated as dangerous goods.

### IMDG

Not regulated as dangerous goods.

**Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code** Not established.

## 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)**

2-BUTANONE (CAS 78-93-3) 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**

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.

**Drug Enforcement Administration (DEA). List 2, Essential Chemicals (21 CFR 1310.02(b) and 1310.04(f)(2) and Chemical Code Number**

2-BUTANONE (CAS 78-93-3) 6714

**Drug Enforcement Administration (DEA). List 1 & 2 Exempt Chemical Mixtures (21 CFR 1310.12(c))**

2-BUTANONE (CAS 78-93-3) 35 %WV

**DEA Exempt Chemical Mixtures Code Number**

2-BUTANONE (CAS 78-93-3) 6714

**FEMA Priority Substances Respiratory Health and Safety in the Flavor Manufacturing Workplace**

2-BUTANONE (CAS 78-93-3) Low priority

**US state regulations** California Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65): This material is not known to contain any chemicals currently listed as carcinogens or reproductive toxins.

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

2-BUTANONE (CAS 78-93-3)

**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)	No
Canada	Non-Domestic Substances List (NDSL)	Yes
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

Country(s) or region	Inventory name	On inventory (yes/no)*
New Zealand	New Zealand Inventory	No
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	Yes
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

<b>Issue date</b>	27-March-2018
<b>Revision date</b>	17-November-2020
<b>Version #</b>	05
<b>Disclaimer</b>	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.
<b>Revision information</b>	This document has undergone significant changes and should be reviewed in its entirety.