

SAFETY DATA SHEET

1. Identification

Product identifier	5-METHYL-2-PHENYL-2-HEXENAL, NO ANTIOXIDANT
Other means of identification	
BRI Product Code	8561
FEMA number	3199
Synonyms	Benzeneacetaldehyde, a-(3-methylbutylidene)- * Cocal
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	
Address	21 Finance 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	Chemtec (North America)	1-800-424-9300
	Chemtec (International)	1-703-527-3887

2. Hazard(s) identification

Physical hazards	Not classified.
Health hazards	Sensitization, skin Category 1B
Environmental hazards	Not classified.
OSHA defined hazards	Not classified.

Label elements



Signal word	Warning
Hazard statement	May cause an allergic skin reaction.
Precautionary statement	
Prevention	Avoid breathing mist or vapor. Contaminated work clothing must not be allowed out of the workplace. Wear protective gloves.
Response	If on skin: Wash with plenty of water. If skin irritation or rash occurs: Get medical advice/attention. Wash contaminated clothing before reuse.
Storage	Store away from incompatible materials.
Disposal	Dispose of contents/container in accordance with local/regional/national/international 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	%
5-METHYL-2-PHENYL-2-HEXENAL , NO ANTIOXIDANT	Benzeneacetaldehyde, a-(3- methylbutylidene)- Cocal	21834-92-4	100

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

4. First-aid measures

Inhalation	Move to fresh air. Call a physician if symptoms develop or persist.
Skin contact	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.
Eye contact	Rinse with water. Get medical attention if irritation develops and persists.
Ingestion	Rinse mouth. Get medical attention if symptoms occur.
Most important symptoms/effects, acute and delayed	May cause an allergic skin reaction. Dermatitis. Rash.
Indication of immediate medical attention and special treatment needed	Provide general supportive measures and treat symptomatically. 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. Wash contaminated clothing before reuse.

5. Fire-fighting measures

Suitable extinguishing media	Water fog. Foam. Dry chemical powder. Carbon dioxide (CO ₂).
Unsuitable extinguishing media	Do not use water jet as an extinguisher, as this will spread the fire.
Specific hazards arising from the chemical	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	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	No unusual fire or explosion hazards noted.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures	Keep unnecessary personnel away. Keep people away from and upwind of spill/leak. 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.
Methods and materials for containment and cleaning up	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. Absorb in vermiculite, dry sand or earth and place into containers. Following product recovery, flush area with water. Small Spills: 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	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	Store in original tightly closed container. 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 in a cool, well-ventilated area.

8. Exposure controls/personal protection

Occupational exposure limits	No exposure limits noted for ingredient(s).
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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.
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. Suitable gloves can be recommended by the glove supplier.
Other	Wear appropriate chemical resistant clothing. Use of an impervious apron is recommended.
Respiratory protection	In case of insufficient ventilation, wear suitable respiratory equipment.
Thermal hazards	Wear appropriate thermal protective clothing, when necessary.
General hygiene considerations	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

Physical state	Liquid.
Color	light yellow
Odor	cocoa aroma.
Odor threshold	Not available.
pH	Not available.
Melting point/freezing point	Not available.
Initial boiling point and boiling range	537.04 °F (280.58 °C) US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Flash point	230 °F (110 °C) Pensky-Martens or Grabner Miniflash
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	0.00337 mmHg at 20°C; US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Vapor density	6.5 Relative to air; air = 1
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Not available.
Partition coefficient (n-octanol/water)	3.77 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	0.968 - 0.978 g/cm ³
Flammability class	Combustible IIIB estimated
Molecular formula	C ₁₃ H ₁₆ O

Molecular weight 188.26
Specific gravity 0.968 - 0.978 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 No dangerous reaction known under conditions of normal use.
Conditions to avoid 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 No adverse effects due to inhalation are expected.
Skin contact 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 May cause an allergic skin reaction.

Product	Species	Test Results
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5-METHYL-2-PHENYL-2-HEXENAL, NO ANTIOXIDANT (CAS 21834-92-4)

Acute

Oral

Liquid

LD50

Rat

> 2500 mg/kg

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

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

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 May cause an allergic skin reaction.

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.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)

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)

3.77, 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

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)

Not listed.

SARA 304 Emergency release notification

Not regulated.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)

Not listed.

Superfund Amendments and Reauthorization Act of 1986 (SARA)

Hazard categories

Immediate Hazard - Yes
Delayed Hazard - No
Fire Hazard - No
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.

US state regulations

US. California Controlled Substances. CA Department of Justice (California Health and Safety Code Section 11100)

Not listed.

US. Massachusetts RTK - Substance List

Not regulated.

US. New Jersey Worker and Community Right-to-Know Act

Not listed.

US. Pennsylvania Worker and Community Right-to-Know Law

Not listed.

US. Rhode Island RTK

Not regulated.

US. California Proposition 65

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.

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)	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 05-24-2015

Version # 01

Disclaimer 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.