

1. Identification

Product identifier 5-METHYL-2-PHENYL-2-HEXENAL

Other means of identification

BRI Product Code 856

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 | Benzeneacetaldehyde, a-(3-methylbutylidene)-Cocal | 21834-92-4 | 100 |

| Stabilizers | Common name and synonyms | CAS number | % |
|----------------------------|--------------------------|------------|-----|
| Chemical name | | | |
| 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 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 | 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 (CO2). |
| 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. |
| Environmental precautions | 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. |

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).

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) 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

0.003 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 |
|--|---------|--------------|
| 5-METHYL-2-PHENYL-2-HEXENAL (CAS 21834-92-4) | | |
| Acute | | |
| Oral | | |
| <i>Liquid</i> | | |
| 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.

Irritation Corrosion - Skin

5-METHYL-2-PHENYL-2-HEXENAL

100 % OECD 406, 1/2 test animals treated with the 100% test material showed a discrete or patchy erythema. Other test animals showed moderate and confluent erythema at the 1 hour reading.
Result: Irritation noted.
Species: Guinea pig
Organ: Skin
Notes: RIFM

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

Irritation Corrosion - Eye

5-METHYL-2-PHENYL-2-HEXENAL

1 %, mild vessel injection which cleared by the third day of observation. Vehicle Ethanol SDA 39C.

Result: Irritation noted.

Species: Rabbit

Organ: Eye

Observation Period: 7 days

Severity: mild

Notes: RIFM

Respiratory or skin sensitization

Respiratory sensitization Not a respiratory sensitizer.

Skin sensitization May cause an allergic skin reaction.

Skin sensitization

5-METHYL-2-PHENYL-2-HEXENAL

100 % OECD 406, Intradermal induction 5% in Freund's Complete Adjuvant/Water/Arachis oil BP. Topical induction 100%. Topical challenge 75% in Arachis oil BP.

Result: Not sensitizing.

Species: Guinea pig

Organ: Skin

Notes: RIFM

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)

5-METHYL-2-PHENYL-2-HEXENAL

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 regulated.

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

Revision date 12-17-2016

Version # 02

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.