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 Chemtrec (North America) 1-800-424-9300
Chemtrec (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

Material name: 5-METHYL-2-PHENYL-2-HEXENAL, NO ANTIOXIDANT

8561 Version #: 01 Issue date: 05-24-2015
**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.

**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.

**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


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)


Auto-ignition temperature

Not available.

Decomposition temperature

Not available.

Viscosity

Not available.

Other information

Density

0.968 - 0.978 g/cm3

Flammability class

Combustible IIIB estimated

Molecular formula

C13H16O
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.  

<table>
<thead>
<tr>
<th>Product</th>
<th>Species</th>
<th>Test Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>5-METHYL-2-PHENYL-2-HEXENAL, NO ANTIOXIDANT (CAS 21834-92-4)</td>
<td>Oral</td>
<td>LD50 Rat &gt; 2500 mg/kg</td>
</tr>
<tr>
<td>5-METHYL-2-PHENYL-2-HEXENAL, NO ANTIOXIDANT (CAS 21834-92-4)</td>
<td>Liquid</td>
<td>Rat</td>
</tr>
</tbody>
</table>

* 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.  
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)

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.
Material name: 5-METHYL-2-PHENYL-2-HEXENAL, NO ANTIOXIDANT

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.