

# Material Safety Data Sheet

Printed : 09/10/2024

Revised : LSI\_2023-1-CLP from 09/10/2024

## 5-METHYL-2-PHENYL-2-HEXENAL (COCOA HEXANAL)

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1. Product identifier

5-METHYL-2-PHENYL-2-HEXENAL (COCOA HEXANAL)

Product identification : 5-METHYL-2-PHENYL-2-HEXENAL (COCOA HEXANAL) code COCH  
C.A.S number : 21834-92-4 ; ;  
CAS EINECS number :  
EINECS number : 244-602-3  
EC (REACH) number :  
REACH registration number : Exempted ( imported or manufactured <1T/year)

#### 1.2. Relevant identified uses of the substance or mixture and uses advised against

Concentrated aromatic raw material.  
Not intended for personal use in this form or concentration.  
For industrial use only, not for retail sale.

USE : **Perfuming substance ; flavouring substance (according to batches)**

#### 1.3. Details of the supplier of the safety data sheet

Company : SASU DIFFUSIONS AROMATIQUES  
558 allée des Parfums  
Parc d'activités "Les Hauts de Grasse"  
06530 SAINT-CEZAIRE-SUR-SIAGNE  
Tel:+33 (0)4 93 60 82 82  
Fax :+33 (0)4 93 60 82 79  
Web :www.diffusions-aromatiques.fr  
Email :contact@diffusions-aromatiques.fr

#### 1.4. Emergency telephone number

Emergency telephone number 24h/24 - 7d/7: ORFILA (INRS) : +33.(0)1.45.42.59.59

### 2. HAZARD IDENTIFICATION

#### 2.1. Classification of the substance or mixture

GHS Classification :

(RegulationCLP)

SS1 Sensitisation skin 1

H317 - May cause an allergic skin reaction.

#### 2.2. Label elements

GHS Classification :

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(RegulationCLP)



Warning mention : Warning

SS1 Sensitisation skin 1

H317 - May cause an allergic skin reaction.

P280 - Wear protective gloves/protective clothing/eye protection/face protection.

P501 - Dispose of contents/container to ...

P261 - Avoid breathing dust/fume/gas/mist/vapours/spray.

P302+P352 - IF ON SKIN: Wash with plenty of soap and water.

P333+P313 - If skin irritation or rash occurs: Get medical advice/attention.

P363 - Wash contaminated clothing before reuse.

## 2.3. Other hazards

- Endocrine disruptors : No components concerned

**- Contains substances that may cause allergies : 5-Methyl-2-phenyl-2-hexenal**

## 3. COMPOSITION / INFORMATION ON INGREDIENT

### 3.1. Substances

Identification number	Substance	Hazard classes & H-phrases	LCS / M-factors / ATE	Percentage %
CAS# 21834-92-4 EINECS# 244-602-3	5-Methyl-2-phenyl-2-hexenal	SS1B H317		[ 70-100 ]

- Endocrine disruptors : No components concerned

### 3.2. Mixtures

NO CONCERNED

## 4. FIRST AID MEASURES

### 4.1. Description of first aid measures

**General notes:** Take Risk and Safety phrases (section 15) into account.

#### Following inhalation:

Remove from exposure site to fresh air and keep at rest. Obtain medical advice.

#### Following skin contact:

Remove contaminated clothes. Wash thoroughly with water (and soap). Contact physician if symptoms persist.

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## Following eye contact:

Flush immediately with water for at least 15 minutes. Contact physician if symptoms persist.

## Following ingestion:

Rinse mouth with water and obtain medical advice.

## Notes for the doctor:

Treat symptomatically and supportively.

Treatment may vary with condition of victim and specifics of incident.

### 4.2. Most important symptoms and effects, both acute and delayed

No data available

Please note the risk and safety phrases

### 4.3. Indication of any immediate medical attention and special treatment needed

No data available

Please note the risk and safety phrases

## 5. FIRE FIGHTING

### 5.1. Extinguishing media

#### Suitable extinguishing media

Depending on the type of product:

- CO2, dry powder or foam extinguishers
- Water spray or fog to cool the package (if necessary)

#### Unsuitable extinguishing media :

Direct water jet

### 5.2. Special hazards arising from the substance or mixture

**Flammability :** The product is not flammable..

**Prévention:** Do not smoke. Do not use flame near.

In case of fire, may produce toxic fumes of carbon monoxide (CO) or carbon dioxide (CO2). Exposure to decomposition products may cause health hazards. Do not breathe fumes.

### 5.3. Advice for firefighters

#### **Never use a direct water jet.**

Workers should be equipped with suitable protective equipment (respiratory and protective suit).

High temperatures can cause high pressures inside closed packages.

## 6. ACCIDENTAL RELEASE MEASURES

### 6.1. Personal precautions, protective equipment and emergency procedures

- Wear gloves (if possible made of natural rubber) when handling leaks to avoid contact with the skin, body cleansing should be observed in case of contact.

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- Avoid breathing vapours.
  - Follow normal hygiene rules in case of accidental spillage.
  - Ensure adequate ventilation of the workplace after spillage.
- Refer to protective measures listed under headings 7 and 8.

## 6.2. Environmental precautions

Prevent contamination of soil and water, runoff into sewers, gutters, rivers. Notify the authorities if the product enters sewers or public waters.

## 6.3. Methods and material for containment and cleaning up

### Methods of cleaning up:

- Large spills should be contained with sand or diatomaceous earth, pumped and rinsed with water after recovery of the waste in specific labelled plastic drums to be handed over to an approved recovery company.
- Clean the area carefully to eliminate any residual pollution
- Any sorbent used to mop up leaks must be destroyed quickly, according to local regulations, preferably by incineration; cases of spontaneous combustion of cloths soaked in perfumes or aromas are well known. Spills must be contained by appropriate means and the associated waste treated in accordance with the regulations in force.

## 6.4. Reference to other sections

See sections 8 and 13 of this safety data sheet where applicable.

## 7. HANDLING AND STORAGE

### 7.1. Precautions for safe handling

- Wear suitable PPE: gloves (preferably natural rubber) and eye/face protection.
- Handle in well-ventilated areas, ventilated if necessary, at the lowest possible temperature, avoiding dust accumulation.
- Do not smoke. Do not expose to flames or other potential sources of ignition (electrical equipment)
- Observe safety and hygiene standards
- Close the packaging after use.
- Reproduce the labelling if transferring to another container.
- Prevent access by unauthorised persons

### 7.2. Conditions for safe storage, including any incompatibilities

- Store products in their original containers, preferably full and tightly capped, in a cool, dry place. Do not reuse empty containers.
- Keep away from air and light.
- Avoid unnecessary exposure.
- Keep away from food and drink.

### 7.3. Specific end use(s)

Wash hands and other exposed areas with mild soap and water before eating, drinking, smoking and before leaving work.

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## 8. EXPOSURE CONTROLS / PERSONAL PROTECTION

### 8.1. Control parameters

Components with Occupational Exposure Limits (OELs) :  
No data available

### 8.2. Exposure controls

Technical measures: Avoid contact with eyes, skin or clothing. Do not ingest. Avoid contact with food, drink.

Personal protective equipment:

Do not eat, drink or smoke during use.



## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

FORMULA :	<b>C13 H16 O</b>
MOLECULAR WEIGHT :	<b>188.27</b>
SHELF LIFE :	<b>24 months in below conditions, after this time it can be used after control.</b>
Storage conditions :	<b>Store the products in tightly closed cans in a cool, dry place, away from light.</b>
FREEZING POINT :	<b>ND</b>
IGNITION POINT :	<b>ND</b>
IGNITION TEMPERATURE (°C) :	<b>ND</b>
EXPLOSIVE LIMITS :	<b>ND</b>
Appearance :	<b>Liquid</b>
Color :	<b>Colorless to pale-yellow</b>
ODOR :	<b>Sweet, chocolate, green, aldehydic</b>
ASSAY (%GC) :	<b>[Sum of isomers ; &gt;95%]</b>
Relative density (d20/20) :	<b>[0.965 ; 0.981]</b>
Refractive index to 20°C :	<b>[1.529 ; 1.536]</b>
Flash point :	<b>&gt; 100°C</b>
BOILING POINT (°C) :	<b>[290°C ; 291]</b>
ACID VALUE (mg KOH/g) :	<b>&lt;10</b>
Solubility(ies) :	<b>Insoluble in water, soluble in ethanol</b>

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OPTICAL ROTATION (°) : **ND**

Vapor pressure : **ND**

Partition coef (n-octanol/water) : **ND**

MELTING POINT (capillarity) °C : **ND**

PH : **ND**

SPECIFIC GRAVITY (25°C g/cm<sup>3</sup>) :

## 9.2. Other information

No data available

## 10. STABILITY AND REACTIVITY

### 10.1. Reactivity

**Dangerous reactions** : No dangerous reactions known.

### 10.2. Chemical stability

Good stability if storage and handling standards/indications are taken into consideration.

### 10.3. Possibility of hazardous reactions

No dangerous reaction if storage and handling standards/indications are taken into account.

### 10.4. Conditions to avoid

Avoid excessive heat sources (open flame, sparks, etc.)  
Do not heat closed containers.  
Avoid contact with oxidizing agents

### 10.5. Incompatible materials

Data not available

### 10.6. Hazardous decomposition products

**Thermal decomposition / conditions to be avoided**: No decomposition if used according to specifications.

**Dangerous decomposition products**: No dangerous decomposition products known.

## 11. TOXICOLOGICAL INFORMATION

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

- a) Skin corrosion/skin irritation : Refer to heading 2, if applicable  
b) Serious eye damage/eye irritation : Refer to heading 2, if applicable  
c) Respiratory or skin sensitisation : Refer to heading 2, if applicable

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- d) Germ cell mutagenicity : Refer to heading 2, if applicable  
e) Carcinogenicity: Refer to heading 2, if applicable  
f) Reproductive toxicity : Refer to heading 2, if applicable  
g) Specific target organ toxicity (STOT)  
single exposure : Refer to heading 2, if applicable  
h) Specific target organ toxicity (STOT)  
repeated exposure : Refer to heading 2, if applicable  
i) Aspiration hazard : Refer to heading 2, if applicable  
j) Acute toxicity :

LD50 (DERMAL) (mg/kg) : **ND**

LD50 (ORAL) (mg/kg) : **ND**

LC50 (inhalatoire) : **ND**

## 11.2. Information on other hazards

Endocrine disrupting properties: The product does not contain substances identified as having endocrine disrupting properties for human health with a concentration equal to or greater than 0.1% (w/w).

### 11.2.2 Others informations

CMR SUBSTANCES : **Dont' contain CMR substances, category 1A, 1B et 2 of 1272/2008 EC regulation**

## 12. ECOLOGICAL INFORMATION

### 12.1. Toxicity

Do not leave the product, even diluted or in great quantity, penetrate the ground water, water or the drains.

### 12.2. Persistence and degradability

BIODEGRADABILITY : **Not available**

### 12.3. Bioaccumulative potential

Data not available

### 12.4. Mobility in soil

Data not available

### 12.5. Results of PBT and vPvB assessment

Data not available

### 12.6. Endocrine disrupting properties

The product does not contain substances identified as having endocrine disrupting properties for the environment with a concentration equal to or greater than 0.1% (w/w).

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## 12.7. Other adverse effects

Data not available

## 13. DISPOSAL RECOMMENDATIONS

### 13.1. Waste treatment methods

**Product** : Recommendation : Does not have to be evacuated with the refuse . Not to let penetrate in the sewers.

**Not cleaned packing** : Recommendation : Evacuation in accordance with the regulations.

## 14. TRANSPORT INFORMATION

### 14.1. UN number

ADR/ADN/RID : NOT REGULATED

IMDG:NOT REGULATED

IATA :NOT REGULATED

### 14.2. UN proper shipping name

ADR/ADN/RID : NOT REGULATED

IMDG:NOT REGULATED

IATA :NOT REGULATED

### 14.3. Transport hazard class(es)

ADR/ADN/RID : NOT REGULATED

IMDG:NOT REGULATED

IATA :NOT REGULATED

### 14.4. Packing group

ADR/ADN/RID : NOT REGULATED

IMDG:NOT REGULATED

IATA :NOT REGULATED

### 14.5. Environmental hazards

IMDG : NOT REGULATED

### 14.6. Special precautions for user

NO CONCERNED

### 14.7. Maritime transport in bulk according to IMO instruments

NO CONCERNED

## 15. REGULATORY INFORMATION

### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

Valeur ICPE : **0**



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## 15.2. Chemical safety assessment

No chemical safety assessment has been carried out

## 16. OTHER INFORMATION

### Full H sentences text in point 3 :

H317 May cause an allergic skin reaction.

### Acronyms used:

C.A.S: Chemical Abstract Service

TSCA: Toxic Substances Control Act

EINECS: European inventory of existing Commercial Chemical Substances

GHS Global Harmonized System

CLP: Classification and Labelling and Packaging of substances and mixtures

ADR: Agreement Dangerous goods by Road

IMDG: International Maritime Dangerous Goods

IATA: International Air Transport Association

The information contained in this sheet is based on our knowledge of the product concerned at the time of issue.

The information given in this safety data sheet is in accordance with Regulation 1907/2006/EC of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) establishing a European Chemicals Agency, (amended by Regulation 2015/830, 2020/878 (Annex II of REACH), amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94, as well as Council Directive 76/769/EEC, and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC, 200/21/EC and according to Regulation 453/2010/EC of 20 May 2010.

Users' attention is also drawn to the possible risks involved when a product is used for a purpose other than that for which it was designed.

The information provided is based on the current state of our knowledge, but does not constitute a guarantee of the product's properties and does not give rise to a contractual legal relationship.

REVISION DATE : **09/10/2024**