



SAFETY DATA SHEET

INTERNATIONAL FLAVORS & FRAGRANCES

Product OCIMENE TOCO

Print Date 10/18/2024

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SECTION 1. PRODUCT AND COMPANY IDENTIFICATION

Product name : OCIMENE TOCO
Sales Number : 00152172
Cust. Material : 00152172
SDS Number : 300000788132
Product Use Description : Fragrance Ingredient

Company : IFF Inc.
600 Highway 36
Hazlet NJ 07730

Telephone : (732) 264-4500
Telefax : (732) 335-2551
Emergency telephone number : +1 800 424 9300

SECTION 2 HAZARDS IDENTIFICATION

GHS-Classification

Flammable liquids, Category 3
Skin irritation, Category 2
Skin sensitisation, Category 1
Aspiration hazard, Category 1

GHS-Labeling

Symbol(s) : 

Signal word : Danger

Hazard statements : H226: Flammable liquid and vapour.
H304: May be fatal if swallowed and enters airways.
H315: Causes skin irritation.
H317: May cause an allergic skin reaction.

Precautionary statements : P210: Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P261: Avoid breathing mist or vapours.

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P280: Wear protective gloves/ eye protection/ face protection.
P301 + P310: IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P302 + P352: IF ON SKIN: Wash with plenty of soap and water.
P331: Do NOT induce vomiting.
P333 + P313: If skin irritation or rash occurs: Get medical advice/ attention.
P370 + P378: In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

Carcinogenicity:

IARC	MYRCENE	123-35-3
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No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

CAS-No. : 13877-91-3

Hazardous components

Component	CAS-No.
1,3,6-Octatriene, 3,7-dimethyl-	13877-91-3
2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-	10191-41-0

SECTION 4. FIRST AID MEASURES

First aid procedures

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

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

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

Ingestion : Rinse mouth with water and obtain medical advice.

Notes to physician

Risks : May be fatal if swallowed and enters airways.
Causes skin irritation.
May cause an allergic skin reaction.

SECTION 5. FIREFIGHTING MEASURES

Flammable properties

Flash point : 132.80 °F (56.00 °C)

Fire fighting

Suitable extinguishing media : Carbondioxide, dry chemical, foam.

Unsuitable extinguishing media : Do not use a direct waterjet on burning material.

Further information : Standard procedure for chemical fires.

Protective equipment and precautions for firefighters

Specific hazards during firefighting : Water may be ineffective.

Special protective equipment for firefighters : Wear NIOSH approved self-contained breathing apparatus and full protective clothing when fighting fires involving chemicals. Use water spray to cool containers exposed to fire.

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SECTION 6. ACCIDENTAL RELEASE MEASURES

- Personal precautions : Avoid inhalation and contact with skin and eyes. A self-contained breathing apparatus is recommended in case of a major spill.
- Environmental precautions : Keep away from drains, surface- and groundwater and soil.
- Methods for containment /
Methods for cleaning up : Clean up spillage promptly. Remove ignition sources. Provide adequate ventilation. Avoid excessive inhalation of vapours. Gross spillages should be contained by use of sand or inert powder and disposed of according to the local regulations.

SECTION 7. HANDLING AND STORAGE

- Handling : Avoid excessive inhalation of concentrated vapors. Follow good manufacturing practices for housekeeping and personal hygiene. Wash any exposed skin immediately after any chemical contact, before breaks and meals, and at the end of each work period. Contaminated clothing and shoes should be thoroughly cleaned before re-use.
- If appropriate, procedures used during the handling of this material should also be used when cleaning equipment or removing residual chemicals from tanks or other containers, especially when steam or hot water is used, as this may increase vapor concentrations in the workplace air. Where chemicals are openly handled, access should be restricted to properly trained employees.
Keep all heated processes at the lowest necessary temperature in order to minimize emissions of volatile chemicals into the air.
- Advice on protection against fire and explosion : Keep away from ignition sources and naked flame.
- Requirements for storage areas and containers : Store in a cool, dry, ventilated area away from heat sources. Keep containers upright and tightly closed when not in use.

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SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

Components	Listed by	Value type	Exposure limit(s)
Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (4R)-	USA. Workplace Environmental Exposure Levels (WEEL)	8-hr TWA	30 ppm

Engineering measures

Engineering measures : Where feasible, isolate mixing rooms and other areas where this material is used or openly handled. Maintain these areas under negative air pressure relative to the rest of the plant. Where feasible, use closed systems to transfer and process this material

Personal protective equipment

Eye protection : Use tight-fitting goggles, face shield or safety glasses with side shields if eye contact might occur.

Hand protection : Avoid skin contact. Use chemically resistant gloves.

Skin and body protection : Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place.

Respiratory protection : Use local exhaust ventilation around open tanks and other open sources of potential exposures in order to avoid excessive inhalation, including places where this material is openly weighed or measured. In addition, use general dilution ventilation of the work area to eliminate or reduce possible worker exposures. No respiratory protection is required during normal operations in a workplace where engineering controls such as adequate ventilation, etc. are sufficient.

If engineering controls and safe work practices are not sufficient, an approved, properly fitted respirator with organic vapor cartridges or

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canisters and particulate filters should be used:

- a) while engineering controls and appropriate safe work practices and/or procedures are being implemented; or
- b) during short term maintenance procedures when engineering controls are not in normal operation or are not sufficient; or
- c) if normal operational workplace vapor concentration in the air is increased due to heat ;
- d) during emergencies; or
- e) if engineering controls and operational practices are not sufficient to reduce airborne concentrations below an established occupational exposure limit.

Hygiene measures

- : To the extent deemed appropriate, implement pre-placement and regularly scheduled ascertainment of symptoms and spirometry testing of lung function for workers who are regularly exposed to this material.
To the extent deemed appropriate, use an experienced air sampling expert to identify and measure volatile chemicals that could be present in the workplace air to determine potential exposures and to ensure the continuing effectiveness of engineering controls and operational practices to minimize exposure.

Protective measures

- : In December 2003, the National Institute for Occupational Safety and Health ("NIOSH") published an Alert on preventing lung disease in workers who use or make flavorings [NIOSH Publication Number 2004-110].
In August 2004, the United States Flavor and Extract Manufacturers Association (FEMA) issued a report entitled "Respiratory Safety in the Flavor Manufacturing Workplace".
Both of these reports provide recommendations for reducing employee exposure and for medical surveillance in the workplace. The recommendations in these reports are generally applicable to the use of any chemical in the workplace and you are strongly urged to review both of these reports.
The report published by FEMA also contains a list of "high priority" chemicals. If any of these chemicals are present in this product at a concentration $\geq 1.0\%$ due to an intentional addition by IFF, the chemical(s) will be identified in this safety data sheet.

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SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Physical state : liquid
Appearance : CLEAR LIQUID
Colour : colorless

Odour : conforms to standard

Safety data

Flash point : 132.80 °F (56.00 °C)

Vapour pressure : .93 hPa (0.93 hPa)
at 68 °F (20 °C)
Note: Calculated

Relative density (20 °C) : 0.7950 - 0.8030

SECTION 10. STABILITY AND REACTIVITY

Conditions to avoid : Remarks: Direct sources of heat.

Materials to avoid : Remarks: Avoid contact with strong acids, alkali or oxidizing agents.

Chemical stability : Remarks: Presents no significant reactivity hazard, by itself or in contact with water.

Hazardous decomposition products : Note: Carbon monoxide and unidentified organic compounds may be formed during combustion.

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SECTION 11. TOXICOLOGICAL INFORMATION

Acute oral toxicity : Acute toxicity estimate
Dose: 4,794 mg/kg
Method: Calculation method

Acute oral toxicity (Component) : Component: 13877-91-3
LD50 Rat
Dose: 5,000 mg/kg
Method: OECD Test Guideline 401
Remarks: REACH data

Component: 5989-27-5
LD50 Rat
Dose: > 2,000 mg/kg
Method: OECD Test Guideline 423
Remarks: REACH data

Component: 123-35-3
LD50 Rat
Dose: > 5,000 mg/kg
Method: OECD Test Guideline 401
Remarks: REACH data

Acute dermal toxicity (Component) : Component: 13877-91-3
LD50 Rabbit
Dose: > 5,000 mg/kg
Method: OECD Test Guideline 402
Remarks: REACH data

Component: 5989-27-5
LD50 Rabbit
Dose: > 5,000 mg/kg
Remarks: Based on data from similar materials
REACH data

Component: 123-35-3
LD50 Rabbit
Dose: > 5,000 mg/kg
Remarks: REACH data

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Skin irritation (Component) : Component: 13877-91-3
reconstructed human epidermis (RhE)
Classification: Causes skin irritation.
Result: Skin irritation
Method: OECD Test Guideline 439
Exposure time: 0.25 h
Test substance:(undiluted)
Remarks: REACH data
Rabbit
Result: Skin irritation
Exposure time: 24 h

Component: 5989-27-5
Rabbit
Classification: Causes skin irritation.
Result: Skin irritation
Method: OECD Test Guideline 404
Exposure time: 4 h
Test substance:(undiluted)
Remarks: REACH data

Component: 99-86-5
Rabbit
Classification: No skin irritation
Result: No skin irritation
Method: OECD Test Guideline 404
Exposure time: 4 h
Remarks: REACH data

Component: 123-35-3
human
Classification: Irritating to skin.
Result: Skin irritation
Method: EPISKIN Human Skin Model Test
Exposure time: 15 min
Remarks: REACH data

Eye irritation(Component) : Component: 13877-91-3
Chicken eye

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Classification: No eye irritation
Result: No eye irritation
Method: OECD Test Guideline 438
Remarks: REACH data

Component: 5989-27-5
Rabbit
Classification: No eye irritation
Result: No eye irritation
Method: OECD Test Guideline 405
Test substance: (undiluted)
Remarks: REACH data

Component: 99-86-5
Rabbit
Classification: Causes serious eye irritation.
Result: Moderate eye irritation
Remarks: REACH data

Component: 123-35-3
Rabbit
Classification: Irritating to eyes.
Result: Irritating to eyes.
Method: OECD Test Guideline 405
Exposure time: 8 d
Remarks: REACH data

Sensitisation (Component) : Component: 13877-91-3
Local lymph node assay (LLNA) Mouse
Classification: Does not cause skin sensitisation.
Result: Does not cause skin sensitisation.
Method: OECD Test Guideline 429
Remarks: REACH data
Based on data from similar materials

Component: 5989-27-5
Local lymph node assay (LLNA) Mouse
Classification: The product is a skin sensitiser, sub-category 1B.
Result: Causes sensitisation.
Method: OECD Test Guideline 429

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Test substance: 22% in ethanol/DEP (75:25)
Remarks: REACH data

Component: 99-86-5
Local lymph node assay (LLNA) Mouse
Classification: The product is a skin sensitiser, sub-category 1B.
Result: positive
Method: OECD Test Guideline 429
Remarks: REACH data

Component: 123-35-3
LLNA Mouse
Classification: Does not cause skin sensitisation.
Result: Not a skin sensitizer.
Method: OECD 429
Remarks: REACH data

Repeated dose
toxicity(Component)

: Component: 13877-91-3

Component: 5989-27-5
OralRat
NOEL: 600 mg/kg
Lowest observed effect level: 150 mg/kg
Method: OECD Test Guideline 408
Remarks: REACH data

OralMouse
NOEL: 500 mg/kg
Lowest observed effect level: 1,000 mg/kg
Method: OECD Test Guideline 408
Remarks: REACH data

Component: 99-86-5
OralMouse
NOEL: 500 mg/kg
Lowest observed effect level: 1,000 mg/kg
Method: OECD Test Guideline 408
Remarks: Based on data from similar materials
REACH data
OralMouse
NOEL: 600 mg/kg

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Lowest observed effect level: 1,200 mg/kg
Method: OECD Test Guideline 408
Remarks: Based on data from similar materials
REACH data
OralMouse
NOEL: 600 mg/kg
Lowest observed effect level: 150 mg/kg
Method: OECD Test Guideline 408
Remarks: Based on data from similar materials
REACH data
OralRat
NOEL: 5 mg/kg
Lowest observed effect level: 30 mg/kg
Remarks: Based on data from similar materials
REACH data
OralDog
NOEL: 100 mg/kg
Lowest observed effect level: 1,000 mg/kg
Method: OECD Test Guideline 409
Remarks: Based on data from similar materials
REACH data

Component: 123-35-3
OralRat
Number of exposures: 1x /day
Method: OECD 408
Remarks: Based on available data, the classification criteria are not met.
REACH data

Carcinogenicity (Component) : Component: 5989-27-5
Oral Mouse
Method: OECD Test Guideline 451
Oral Mouse
Method: OECD Test Guideline 451

SECTION 12. ECOLOGICAL INFORMATION

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Component:

13877-91-3

OCIMENE

Toxicity to daphnia and other aquatic invertebrates:

semi-static test EC50

Species: Daphnia magna (Water flea)

Dose: 1.47 mg/l

Exposure time: 48 h

Analytical monitoring: yes

Method: OECD Test Guideline 202

Based on data from similar materials

REACH data

Toxicity to algae:

static test EC50

Species: Pseudokirchneriella subcapitata (green algae)

Dose: 0.342 mg/l

Exposure time: 48 h

Analytical monitoring: yes

Method: OECD Test Guideline 201

Based on data from similar materials

REACH data

5989-27-5

Limonene,D-
(5989-27-5)

Toxicity to fish:

flow-through test LC50

Species: Pimephales promelas (fathead minnow)

Dose: 0.720 mg/l

Exposure time: 96 h

Analytical monitoring: yes

Method: OECD Test Guideline 203

REACH data

Toxicity to daphnia and other aquatic invertebrates:

semi-static test EC50

Species: Daphnia magna (Water flea)

Dose: 0.307 mg/l

Exposure time: 48 h

Analytical monitoring: yes

Method: OECD Test Guideline 202

REACH data

Toxicity to algae:

static test EC50

Species: Raphidocelis subcapitata (freshwater green alga)

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Dose: 0.32 mg/l
Exposure time: 72 h
Analytical monitoring: yes
Method: OECD Test Guideline 201
REACH data
Toxicity to algae:
static test EC10
Species: Raphidocelis subcapitata (freshwater green alga)
Dose: 0.174 mg/l
Exposure time: 72 h
Analytical monitoring: yes
Method: OECD Test Guideline 201
REACH data
Toxicity to bacteria:
static test EC50
Species: activated sludge
Dose: 209 mg/l
Exposure time: 3 h
Analytical monitoring: no
Method: OECD Test Guideline 209
REACH data
Toxicity to bacteria:
static test EC10
Species: activated sludge
Dose: 18 mg/l
Exposure time: 3 h
Analytical monitoring: no
Method: OECD Test Guideline 209
REACH data
<03EHS L TEXT(CED-N12.00224460)>
<03EHS L TEXT(CED-H11.00000120)>;
semi-static test NOEC
Species: Pimephales promelas (fathead minnow)
Concentration: .37 mg/l
Exposure time: 8 d
Analytical monitoring: yes
Remarks:
REACH data
<03EHS L TEXT(CED-H12.00200010)>

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<03EHS L TEXT(CED-H11.00000120)>:

semi-static test EC10

Species: Daphnia magna (Water flea)

Concentration: .15 mg/l

Exposure time: 21 d

Analytical monitoring: yes

Method: OECD Test Guideline 211

Remarks:

REACH data

<03EHS L TEXT(CED-H12.00200010)>

<03EHS L TEXT(CED-H11.00000120)>:

semi-static test NOEC

Species: Daphnia magna (Water flea)

Concentration: .08 mg/l

Exposure time: 21 d

Analytical monitoring: yes

Method: OECD Test Guideline 211

Remarks:

REACH data

99-86-5

Terpinene alpha

Toxicity to fish:

flow-through test LC50

Species: Pimephales promelas (fathead minnow)

Dose: ca. 3.150 mg/l

Exposure time: 96 h

Analytical monitoring: yes

Method: OECD Test Guideline 203

REACH data

Toxicity to daphnia and other aquatic invertebrates:

semi-static test EC50

Species: Daphnia magna (Water flea)

Dose: 1.7 mg/l

Exposure time: 48 h

Analytical monitoring: yes

Method: OECD Test Guideline 202

REACH data

Toxicity to daphnia and other aquatic invertebrates:

semi-static test NOEC

Species: Daphnia magna (Water flea)

Dose: 0.97 mg/l

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Exposure time: 48 h
Analytical monitoring: yes
Method: OECD Test Guideline 202
REACH data
Toxicity to algae:
static test NOEC
Species: Raphidocelis subcapitata (freshwater green alga)
Dose: 3.7 mg/l
Exposure time: 72 h
Analytical monitoring: yes
Method: OECD Test Guideline 201
REACH data
Toxicity to bacteria:
static test EC50
Species: activated sludge
Dose: > 1,000 mg/l
Exposure time: 3 h
Analytical monitoring: no
Method: OECD Test Guideline 209

123-35-3

MYRCENE

Toxicity to fish:
semi-static test LC50
Species: Cyprinus carpio (Carp)
Dose: 0.46 mg/l
Exposure time: 96 h
Method: OECD Test Guideline 203
REACH data
Toxicity to daphnia and other aquatic invertebrates:
semi-static test
Species: Daphnia magna (Water flea)
Dose: 1.47 mg/l
Exposure time: 48 h
Method: OECD Test Guideline 202
REACH data
Toxicity to algae:
static test
Species: Pseudokirchneriella subcapitata (green algae)
Dose: 0.342 mg/l

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Exposure time: 76 h
Method: OECD Test Guideline 201
REACH data

SECTION 13. DISPOSAL CONSIDERATIONS

Contaminated packaging : Place material into sealed containers and dispose of in accordance with local, state and federal regulations.

SECTION 14. TRANSPORT INFORMATION

DOT Proper shipping name : Combustible liquid, n.o.s.
(3,7-DIMETHYL-1,3,6-OCTATRIENE)
Labels : NONE
UN number : 1993
Class : CBL
Packing group : III
Emergency Response : 128
Guidebook Number

DOT NON-BULK Not dangerous goods

IATA UN number : 1993
Description of the goods : FLAMMABLE LIQUID, N.O.S.
(3,7-DIMETHYL-1,3,6-OCTATRIENE)
Class : 3
Packing group : III
ICAO-Labels : 3

IMDG UN number : 1993
Description of the goods : FLAMMABLE LIQUID, N.O.S.
(3,7-DIMETHYL-1,3,6-OCTATRIENE)
Class : 3
Packing group : III
IMDG-Labels : 3
EmSNumber 1 : F-E
EmSNumber 2 : S-E

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Marine pollutant : yes
(3,7-DIMETHYL-1,3,6-OCTATRIENE)

Other information : Above applies only to containers over 119 gallons or 450 liters. Not regulated if shipped in packages less than or equal to 119 gallons (450 liters). If transporting by vessel or aircraft, unless other means of transportation is impracticable, then the product must be shipped as a flammable liquid.

SECTION 15. REGULATORY INFORMATION

SARA 311/312 Hazards : Flammable (gases, aerosols, liquids, or solids)
Skin corrosion or irritation
Aspiration hazard
Respiratory or skin sensitisation

Reportable Quantity :

HMIS Classification : Health hazard: 1
Chronic Health Hazard: /
Flammability: 2
Physical and chemical hazards: 0

SECTION 16. OTHER INFORMATION

Further information

The information in this MSDS was obtained from current and reliable sources. However the data is provided without any warrant, expressed or implied, regarding its correctness or accuracy. Since the use, handling, storage and disposal of this product are beyond IFF control, it is the responsibility of the user both to determine safe conditions for the use of this product and to assume liability of loss, damage, or expense arising out of the product's improper use. No warranty expressed or implied regarding the product described herein shall be created by or inferred from any statement or omission in this MSDS. Various Federal, State or Provincial agencies may have specific regulations concerning the transportation, handling, storage, use, or disposal of this product which may not be reflected in this MSDS. The user should review these regulations to ensure full compliance.

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