



# SAFETY DATA SHEET

## INTERNATIONAL FLAVORS & FRAGRANCES

Product FLEURANIL

Print Date 04.11.2019

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### 1. Identification of the substance/mixture and of the company/undertaking

#### 1.1 Product identifier

Trade name : FLEURANIL  
Registration number : 01-0000015990-66-0000  
IFF Code : 00062144  
SDS Number : R00000221523  
Substance name : reaction mass of: 3-(4-ethylphenyl)-2,2-dimethylpropanenitrile; 3-(2-ethylphenyl)-2,2-dimethylpropanenitrile; 3-(3-ethylphenyl)-2,2-dimethylpropanenitrile  
Substance No. : 412-660-0

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

Use of the Substance/Mixture : Ingredient used in Flavour and/or Fragrance preparations

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

Company : IFF Benicarló, S.L.  
Avda. Felipe Klein 2  
12580 BENICARLÓ  
Spain  
Telephone : +34964470212  
Telefax : +34964473411  
E-mail address : sds@iff.com  
Responsible/issuing person

#### 1.4 Emergency telephone number

Refer to section 16 for country specific emergency contact number.

### 2. Hazards identification

#### 2.1 Classification of the substance or mixture

##### Classification (REGULATION (EC) No 1272/2008)

Chronic aquatic toxicity, Category 2 H411: Toxic to aquatic life with long lasting effects.

#### 2.2 Label elements

##### Labelling (REGULATION (EC) No 1272/2008)

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Hazard pictograms

:



Hazard statements

: H411

Toxic to aquatic life with long lasting effects.

Precautionary statements

: **Prevention:**

P273

Avoid release to the environment.

**Response:**

P391

Collect spillage.

**Disposal:**

P501

Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Other hazards

None reasonably foreseeable.

## 3. Composition/information on ingredients

### 3.1 Substances

Chemical name of the substance : reaction mass of: 3-(4-ethylphenyl)-2,2-dimethylpropanenitrile; 3-(2-ethylphenyl)-2,2-dimethylpropanenitrile; 3-(3-ethylphenyl)-2,2-

Chemical characterization : aromatic nitriles

Molecular formula : C<sub>13</sub>H<sub>17</sub>N

Molecular weight : 187,14 g/mol

CAS-No. : 134123-93-6

EINECS-No. : 412-660-0

REACH No. : 01-0000015990-66-0000

#### Hazardous components

Chemical name	CAS-No. EC-No.	GHS Classification	Concentration [%]
reaction mass of: 3-(4-ethylphenyl)-2,2-	134123-93-6 412-660-0	Aquatic Chronic2; H411	90 - 100

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dimethylpropanenitrile; 3-(2-ethylphenyl)-2,2-dimethylpropanenitrile; 3-(3-ethylphenyl)-2,2-dimethylpropanenitrile	412-660-0		
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For the full text of the H-Statements mentioned in this Section, see Section 16.

### 3.2 Mixtures

Not applicable, product is a substance.

## 4. First aid measures

### 4.1 Description of first aid measures

- General advice : Take Hazard and Precautionary phrases (section 2) into account.
- If inhaled : Remove from exposure site to fresh air and keep at rest. If victim is unconscious, remove foreign bodies from the mouth. If victim has stopped breathing, give artificial respiration. Obtain medical advice.
- In case of skin contact : Remove contaminated clothes. Wash thoroughly with water (and soap). Contact physician if symptoms persist.
- In case of eye contact : Flush immediately with water for at least 15 minutes. Contact physician if symptoms persist.
- If swallowed : Rinse mouth with water and obtain medical advice.

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

- Symptoms : No information available.
- Risks : No information available.

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

- Treatment : No information available.

## 5. Firefighting measures

### 5.1 Extinguishing media

- Suitable extinguishing media : Carbondioxide, dry chemical, foam.

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

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

Specific hazards during firefighting : Water may be ineffective.

### 5.3 Advice for firefighters

Further information : Standard procedure for chemical fires.

## 6. Accidental release measures

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

Personal precautions : Avoid inhalation and contact with skin and eyes. A self-contained breathing apparatus is recommended in case of a major spill.

### 6.2 Environmental precautions

Environmental precautions : Keep away from drains, surface- and groundwater and soil.

### 6.3 Methods and materials for containment and cleaning up

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.

### 6.4 Reference to other sections

Prevent spreading over a wide area (e.g. by containment or oil barriers).

## 7. Handling and storage

### 7.1 Precautions for safe handling

Advice on safe 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.

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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.

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

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.

### 7.3 Specific end use(s)

Specific use(s) : No information available.

## 8. Exposure controls/personal protection

### 8.1 Control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Engineering measures

Where appropriate, use closed systems to transfer and process this material.  
If appropriate, 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.

#### Personal protective equipment

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,

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etc. are sufficient.

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

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

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

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.

### Environmental exposure controls

General advice : Keep away from drains, surface- and groundwater and soil.

## 9. Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

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Appearance : liquid  
Colour : colorless  
Odour : conforms to standard  
Odour Threshold : not determined  
Flash point : 132 °C  
Lower explosion limit : not determined  
Upper explosion limit : not determined  
Flammability (solid, gas) : not determined  
Oxidizing properties : not determined  
Auto-ignition temperature : 405 °C  
pH : not determined  
Melting point : -37 °C  
Boiling point : 263 - 278 °C  
Vapour pressure : 0,02 hPa Calculated  
  
Density : not determined  
Water solubility : 0,083 g/l at 20 °C  
  
Partition coefficient: n-octanol/water : log Pow: 3,460 at 22 °C  
Solubility in other solvents : not determined  
Viscosity, dynamic : not determined  
Viscosity, kinematic : not determined  
Relative vapour density : not determined  
Surface tension : 61,2 mN/m  
at 20 °C  
  
Evaporation rate : not determined

### 9.2 Other information

Refractive index : not determined  
Relative density : 0,9390 - 0,9460

## 10. Stability and reactivity

### 10.1 Reactivity

No hazards to be specially mentioned.

### 10.2 Chemical stability

Stable under normal conditions.

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### 10.3 Possibility of hazardous reactions

Hazardous reactions : Note: Presents no significant reactivity hazard, by itself or in contact with water. Avoid contact with strong acids, alkali or oxidizing agents.

### 10.4 Conditions to avoid

Conditions to avoid : Direct sources of heat.

### 10.5 Incompatible materials

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

### 10.6 Hazardous decomposition products

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

## 11. Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Acute oral toxicity : LD50: > 2.000 mg/kg  
Species: Rat

Acute dermal toxicity : LD50: > 2.000 mg/kg  
Species: Rat

#### Skin corrosion/irritation

Skin irritation : No information available.  
Skin irritation : Species: Rabbit  
Result: Skin irritation  
Exposure time: 24 h

#### Serious eye damage/eye irritation

No information available.  
Eye irritation : Species: Rabbit  
Result: Mild eye irritation  
Exposure time: 24 h

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Test substance: (undiluted)

### Respiratory or skin sensitisation

No information available.

Sensitisation

: Species: human

Result: Did not cause sensitisation on laboratory animals.

Test substance: 6.0% in ethanol

: Species: Guinea pig

Result: Did not cause sensitisation on laboratory animals.

Test substance: 0.0%

### Germ cell mutagenicity

No information available.

### Carcinogenicity

No information available.

### Reproductive toxicity

No information available.

### Target Organ Systemic Toxicant - Single exposure

No information available.

### Target Organ Systemic Toxicant - Repeated exposure

No information available.

### Aspiration hazard

No information available.

## 12. Ecological information

### 12.1 Toxicity

Toxicity to fish

: LC50: 6,2 mg/l

Exposure time: 96 h

Method: OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

: EC50: 5,3 mg/l

Exposure time: 48 h

Method: OECD Test Guideline 202

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Toxicity to algae : EbC50: 6,3 mg/l  
Exposure time: 72 h  
Method: OECD Test Guideline 201

: ErC50: 11,2 mg/l  
Exposure time: 72 h  
Method: OECD Test Guideline 201

### 12.2 Persistence and degradability

No information available.

Biodegradability : Result: Not readily biodegradable.  
6 %  
Method: Directive 67/548/EEC Annex V, C.4.D.

### 12.3 Bioaccumulative potential

No information available.

### 12.4 Mobility in soil

### 12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

### 12.6 Other adverse effects

No information available.

## 13. Disposal considerations

### 13.1 Waste treatment methods

Product : Dispose of according to local regulations. Avoid disposing into drainage systems and into the environment.

Contaminated packaging : Empty containers should be taken to an approved waste handling site for recycling or disposal.

## 14. Transport information

### ADR

UN number : 3082

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Description of the goods : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.  
(4-ETHYL-DIMETHYLBENZENEPROPANENITRILE)

Labels : 9

Packing group : III

Environmentally hazardous : yes

**IATA**

UN number : 3082

Description of the goods : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.  
(4-ETHYL-DIMETHYLBENZENEPROPANENITRILE)

Labels : 9

Packing group : III

Environmentally hazardous : yes

**IMDG**

UN number : 3082

Description of the goods : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.  
(4-ETHYL-DIMETHYLBENZENEPROPANENITRILE)

Labels : 9

Packing group : III

Marine pollutant : yes (4-ETHYL-DIMETHYLBENZENEPROPANENITRILE)

**Special precautions for user** : No special precautions required.

### 15. Regulatory information

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

Water contaminating class : WGK 2 significantly water endangering  
(Germany)

#### 15.2 Chemical safety assessment

A Chemical Safety Assessment is not required for this substance.

### 16. Other information

#### Full text of H-Statements referred to under sections 2 and 3.

H411 Toxic to aquatic life with long lasting effects.

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### Further information

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.

According to Regulation (EC) No. 1907/2006 the information in this safety data sheet is based on the properties of the material known to IFF at the time the data sheet was issued. The safety data sheet is intended to provide information for a health and safety assessment of the material and the circumstances, under which it is packaged, stored or applied in the workplace. For such a safety assessment International Flavors & Fragrances holds no responsibility. This document is not intended for quality assurance purposes.

### Emergency telephone number

Austria	+43 1 406 43 43
Belgium	+32 70 245 245
Bulgaria	+359 2 9154 409 (N. I. Pirogov). <a href="mailto:poison_centre@mail.orbitel.bg">poison_centre@mail.orbitel.bg</a>
Croatia	(+385 1) 2348342
Czech Republic	+420 224 919 293 / +420 224 915 402
Denmark	+45 82 12 12 12
Estonia	16662 (National), International (+372) 626 93 90
Finland	+358 9 471977
France	+ 33 (0)1 45 42 59 59
Germany	+31 13 4642 211
Greece	+31 13 4642 211
Hungary	(+36-80) 201-199
Iceland	+354 543 2222
Ireland	+353 1 8092566 / +353 1 8379964
Italy	+39 06 68593726
Latvia	+371 67042473
Lithuania	+370 5 236 20 52 or +370 687 53378

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Luxembourg	+352 8002 5500
Malta	+356 21224071
Netherlands	+31 30 2748888 (Only for the purpose of informing medical personnel in cases of acute intoxications).
Norway	+47 22 59 13 00
Poland	+31 13 4642 211
Portugal	808 250 143
Poland	+31 13 4642 211
Portugal	808 250 143
Romania	+31 13 4642 211
Slovakia	+31 13 4642 211
Slovenia	+31 13 4642 211
Spain	+34 91 562 04 20 (only for the purpose of informing medical personnel in cases of acute intoxications).
Sweden	+46 112
United Kingdom	+44 111 (England, Wales & Scotland)

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Classification: **Internal**