

## Chemical Safety Data Sheet MSDS / SDS

**(E)-3-[3'-(4''-Fluorophenyl)-1'-(1''-methylethyl)-1H-indol-2''-yl]-2-propnal**

Revision Date:2023-12-07 Revision Number:1

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : (E)-3-[3'-(4''-Fluorophenyl)-1'-(1''-methylethyl)-1H-indol-2''-yl]-2-propnal  
CBnumber : CB8855583  
CAS : 93957-50-7  
EINECS Number : 425-370-4  
Synonyms : (E)-3-(3-(4-fluorophenyl)-1-isopropyl-1H-indol-2-yl)acrylaldehyde,(E)-3-[3'-(4''-Fluorophenyl)-1'-(1''-methylethyl)-1H-indol-2''-yl]-2-propnal

**Relevant identified uses of the substance or mixture and uses advised against**

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 400-158-6606

**SECTION 2: Hazards identification****Classification of the substance or mixture**

Skin sensitization, Category 1  
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

**Label elements****Pictogram(s)**

Signal word : Warning

**Hazard statement(s)**

H317 May cause an allergic skin reaction  
H410 Very toxic to aquatic life with long lasting effects

**Precautionary statement(s)****Prevention**

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

P272 Contaminated work clothing should not be allowed out of the workplace.

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

P273 Avoid release to the environment.

#### Response

P302+P352 IF ON SKIN: Wash with plenty of water/...

P333+P317 If skin irritation or rash occurs: Get medical help.

P321 Specific treatment (see ... on this label).

P362+P364 Take off contaminated clothing and wash it before reuse.

P391 Collect spillage.

#### Storage

none

#### Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

#### Other hazards

no data available

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## SECTION 3: Composition/information on ingredients

#### Substance

Product name	: (E)-3-[3'-(4"-Fluorophenyl)-1'-(1"-methylethyl)-1H-indol-2"-yl]-2-propnal
Synonyms	: (E)-3-(3-(4-fluorophenyl)-1-isopropyl-1H-indol-2-yl)acrylaldehyde,(E)-3-[3'-(4"-Fluorophenyl)-1'-(1"-methylethyl)-1H-indol-2"-yl]-2-propnal
CAS	: 93957-50-7
EC number	: 425-370-4
MF	: C20H18FNO
MW	: 307.36

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## SECTION 4: First aid measures

#### Description of first aid measures

##### If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately.

Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

##### Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

##### Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

##### Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control

Center immediately.

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

no data available

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

no data available

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## SECTION 5: Firefighting measures

### Extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam.

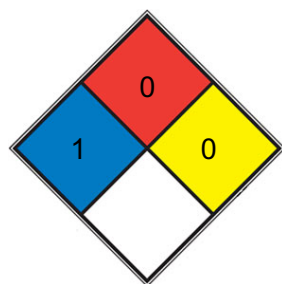
### Specific Hazards Arising from the Chemical

no data available

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### NFPA 704



■ HEALTH 1 Exposure would cause irritation with only minor residual injury (e.g. [acetone](#), sodium bromate, potassium chloride)

■ FIRE 0 Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes.(e.g. Carbon tetrachloride)

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,[N2](#))

□ SPEC.

□ HAZ.

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## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours.Avoid contacting with skin and eye. Use personal protective equipment.Wear chemical impermeable gloves. Ensure adequate ventilation.Remove all sources of ignition. Evacuate personnel to safe areas.Keep people away from and upwind of spill/leak.

## Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

## Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

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# SECTION 7: Handling and storage

## Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

## Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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# SECTION 8: Exposure controls/personal protection

## Control parameters

### Occupational Exposure limit values

no data available

### Biological limit values

no data available

## Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

## Individual protection measures

### Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

### Skin protection

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

### Thermal hazards

no data available

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# SECTION 9: Physical and chemical properties

## Information on basic physicochemical properties

Physical state	Solid. Powder.
Colour	no data available
Odour	no data available
Melting point/freezing point	128 - 129 °C.
Boiling point or initial boiling point and boiling range	106°C/13mmHg(lit.)
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	87°C(lit.)
Auto-ignition temperature	> 400 °C.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	In water: 0.08 mg/L. Temperature:20 °C. pH:Ca. 5.5.
Partition coefficient n-octanol/water	log Pow = 4.5. Temperature:27 °C.
Vapour pressure	0.204 Pa. Temperature:38.13 °C.;0.103 Pa. Temperature:30.85 °C.;0.06 Pa. Temperature:24.82 °C.
Density and/or relative density	1.27. Temperature:20 °C.
Relative vapour density	no data available
Particle characteristics	no data available

## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

no data available

### Possibility of hazardous reactions

no data available

### Conditions to avoid

no data available

### Incompatible materials

no data available

### Hazardous decomposition products

no data available

## SECTION 11: Toxicological information

### Acute toxicity

- Oral: LD50 - (male/female) - > 2 000 mg/kg bw.
- Inhalation: no data available
- Dermal: LD50 - (male/female) - > 2 000 mg/kg bw.

### Skin corrosion/irritation

no data available

### Serious eye damage/irritation

no data available

### Respiratory or skin sensitization

no data available

### Germ cell mutagenicity

no data available

### Carcinogenicity

no data available

### Reproductive toxicity

no data available

### STOT-single exposure

no data available

### STOT-repeated exposure

no data available

### Aspiration hazard

no data available

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## SECTION 12: Ecological information

### Toxicity

Toxicity to fish: LC50 - 0.047 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - other aquatic crustacea: - 0.064 mg/L - 48 h.

Toxicity to algae: EC50 - *Pseudokirchneriella subcapitata* (previous names: *Raphidocelis subcapitata*, *Selenastrum capricornutum*) - 0.016 mg/L - 72 h.

Toxicity to microorganisms: IC50 - > 100 mg/L.

### Persistence and degradability

no data available

### **Bioaccumulative potential**

no data available

### **Mobility in soil**

no data available

### **Other adverse effects**

no data available

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## **SECTION 13: Disposal considerations**

### **Disposal methods**

#### **Product**

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

#### **Contaminated packaging**

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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## **SECTION 14: Transport information**

### **UN Number**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **UN Proper Shipping Name**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Transport hazard class(es)**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Packing group, if applicable**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

## Environmental hazards

ADR/RID: Yes

IMDG: Yes

IATA: Yes

## Special precautions for user

no data available

## Transport in bulk according to IMO instruments

no data available

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# SECTION 15: Regulatory information

## Safety, health and environmental regulations specific for the product in question

### European Inventory of Existing Commercial Chemical Substances (EINECS)

Not Listed.

### EC Inventory

Not Listed.

### United States Toxic Substances Control Act (TSCA) Inventory

Not Listed.

### China Catalog of Hazardous chemicals 2015

Not Listed.

### New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

### PICCS

Not Listed.

### Vietnam National Chemical Inventory

Not Listed.

### IECSC

Not Listed.

### Korea Existing Chemicals List (KECL)

Not Listed.

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# SECTION 16: Other information

## Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association



TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

## References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: [http://www.echemportal.org/echemportal/index?pagelD=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pagelD=0&request_locale=en)

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

### Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.