

## Chemical Safety Data Sheet MSDS / SDS

## 5-allyl-1,3-benzodioxole SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: 5-allyl-1,3-benzodioxole

CAS: 94-59-7

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

Relevant identified uses: For R&amp;D use only. Not for medicinal, household or other use.

Uses advised against: none

**Company Identification**

Company: Chemicalbook.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

Telephone: +91 9550333722

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

Acute toxicity - Category 4, Oral

Germ cell mutagenicity, Category 2

Carcinogenicity, Category 1B

**GHS label elements, including precautionary statements**

Pictogram(s)



Signal word

Danger

**Hazard statement(s)**

H302 Harmful if swallowed

H341 Suspected of causing genetic defects

H350 May cause cancer

**Precautionary statement(s)**

**Prevention**

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P203 Obtain, read and follow all safety instructions before use.

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

**Response**

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P318 IF exposed or concerned, get medical advice.

**Storage**

P405 Store locked up.

**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 which do not result in classification**

no data available

### SECTION 3: Composition/information on ingredients

#### Substance

Chemical name:	5-allyl-1,3-benzodioxole
Common names and synonyms:	5-allyl-1,3-benzodioxole
CAS number:	94-59-7
EC number:	202-345-4
Concentration:	100%

### SECTION 4: First aid measures

#### Description of necessary 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/effects, acute and delayed

SYMPTOMS: This compound can cause vomiting, shock, cyanosis, delirium and probably convulsions. ACUTE/CHRONIC HAZARDS: This material will cause severe irritation if ingested. (NTP, 1992)

##### Indication of immediate medical attention and special treatment needed, if necessary

Treatment for acute oil of sassafras ingestion is supportive and includes administration of oral activated charcoal, support of respiration and circulation, and adequate fluid and electrolyte replacement.

## SECTION 5: Firefighting measures

### Suitable extinguishing media

Fires involving this compound should be controlled using a dry chemical, carbon dioxide or Halon extinguisher. (NTP, 1992)

### Specific hazards arising from the chemical

This chemical is combustible. (NTP, 1992)

### Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

## 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

PRECAUTIONS FOR "CARCINOGENS": A high-efficiency particulate arrestor (HEPA) or charcoal filters can be used to minimize amt of carcinogen in exhausted air ventilated safety cabinets, lab hoods, glove boxes or animal rooms ... Filter housing that is designed so that used filters can be transferred into plastic bag without contaminating maintenance staff is avail commercially. Filters should be placed in plastic bags immediately after removal ... The plastic bag should be sealed immediately ... The sealed bag should be labelled properly ... Waste liquids ... should be placed or collected in proper containers for disposal. The lid should be secured & the bottles properly labelled. Once filled, bottles should be placed in plastic bag, so that outer surface ... is not contaminated ... The plastic bag should also be sealed & labelled. ... Broken glassware ... should be decontaminated by solvent extraction, by

chemical destruction, or in specially designed incinerators. Chemical Carcinogens

## 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

PRECAUTIONS FOR "CARCINOGENS": Storage site should be as close as practical to lab in which carcinogens are to be used, so that only small quantities required for ... expt need to be carried. Carcinogens should be kept in only one section of cupboard, an explosion-proof refrigerator or freezer (depending on chemico-physical properties ...) that bears appropriate label. An inventory ... should be kept, showing quantity of carcinogen & date it was acquired ... Facilities for dispensing ... should be contiguous to storage area. Chemical Carcinogens

## SECTION 8: Exposure controls/personal protection

### Control parameters

### Occupational Exposure limit values

no data available

### Biological limit values

no data available

### Appropriate engineering 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, such as personal protective equipment (PPE)

#### Eye/face protection

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

#### Skin protection

Wear fire/flame 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

### **SECTION 9: Physical and chemical properties and safety characteristics**

Physical state:	PHYSICAL DESCRIPTION: Clear colorless or slightly yellow liquid with the odor of sassafras. Denser than water (density 1.09 g / cm <sup>3</sup> ) and insoluble in water. Hence sinks in water. Obtained from oil of sassafras or oil of camphor.
Colour:	Colorless or pale yellow oil
Odour:	Sassafras odor
Melting point/freezing point:	11 °C
Boiling point or initial boiling point and boiling range:	232 - 234C
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	97 °C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available

pH:	no data available
Kinematic viscosity:	no data available
Solubility:	less than 1 mg/mL at 64° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Kow = 3.45/Estimated/
Vapour pressure:	1 mm Hg ( 63.8 °C)
Density and/or relative density:	1.09
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

Slight. SAFROLE, an acetal, is readily hydrolyzed in acidic solution to give 4-allylpyrocatechol and formaldehyde (or formaldehyde polymers).

### Conditions to avoid

no data available

### Incompatible materials

Combustible when exposed to heat or flame.

#### **Hazardous decomposition products**

When heated to decomposition it emits acrid smoke and irritating fumes.

### **SECTION 11: Toxicological information**

#### **Acute toxicity**

Oral: LD50 Rat oral 1950 mg/kg

Inhalation: no data available

Dermal: no data available

#### **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**

The Human Health Assessment Group in EPA's Office of Health and Environmental Assessment has evaluated safrole for carcinogenicity. According to their analysis, the weight-of-evidence for safrole is group B2, which is based on sufficient evidence in animals. No data are available in humans. As a group B2 chemical, safrole is considered probably carcinogenic to humans.

#### **Reproductive toxicity**

no data available



**STOT-single exposure**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

**SECTION 12: Ecological information****Toxicity**

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

**Persistence and degradability**

no data available

**Bioaccumulative potential**

An estimated BCF of 90 was calculated for safrole(SRC), using an estimated log Kow of 3.45(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is moderate(SRC).

**Mobility in soil**

Using a structure estimation method based on molecular connectivity indices(1), the Koc for safrole can be estimated to be 300(SRC). According to a classification scheme(2), this estimated Koc value suggests that safrole is expected to have moderate mobility in soil.

### **Other adverse effects**

no data available

## **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.

## **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: No  
IMDG: No  
IATA: No

#### **Special precautions for user**

no data available

#### **Transport in bulk according to IMO instruments**

no data available

### **SECTION 15: Regulatory information**

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

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

Listed.

##### **EC Inventory**

Listed.

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

Listed.

##### **China Catalog of Hazardous chemicals 2015**

Not Listed.

##### **New Zealand Inventory of Chemicals (NZIoC)**

Listed.

##### **(PICCS)**

Listed.

**Vietnam National Chemical Inventory**

Listed.

**IECSC)**

Listed.

**Korea Existing Chemicals List (KECL)**

Listed.

## **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?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=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/>

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