

### 1. PRODUCT AND COMPANY IDENTIFICATION

Product name	:	Safrole	
Product Number	:	S9652	
Brand	:	Sigma	
Product Use	:	For laboratory research purposes.	
Supplier	:	Sigma-Aldrich Canada Co. 2149 Winston Park Drive OAKVILLE ON L6H 6J8 CANADA	Manufacturer : Sigma-Aldrich Corporation 3050 Spruce St. St. Louis, Missouri 63103 USA
Telephone	:	+1 9058299500	
Fax	:	+1 9058299292	
Emergency Phone # (For both supplier and manufacturer)	:	1-800-424-9300	
Preparation Information	:	Sigma-Aldrich Corporation Product Safety - Americas Region 1-800-521-8956	

### 2. HAZARDS IDENTIFICATION

#### Emergency Overview

#### Target Organs

Liver

#### WHMIS Classification

D2A	Very Toxic Material Causing Other Toxic Effects	Carcinogen
D2B	Toxic Material Causing Other Toxic Effects	Moderate skin irritant Mutagen

#### GHS Classification

Acute toxicity, Oral (Category 4)  
Skin irritation (Category 2)  
Germ cell mutagenicity (Category 2)  
Carcinogenicity (Category 1B)

#### GHS Label elements, including precautionary statements

Pictogram



Signal word                      Danger

Hazard statement(s)

H302	Harmful if swallowed.
H315	Causes skin irritation.
H341	Suspected of causing genetic defects.
H350	May cause cancer.

Precautionary statement(s)

P201	Obtain special instructions before use.
P281	Use personal protective equipment as required.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.

**HMIS Classification**

Health hazard: 2  
Chronic Health Hazard: \*  
Flammability: 1  
Physical hazards: 0

**Potential Health Effects**

**Inhalation** May be harmful if inhaled. Causes respiratory tract irritation.  
**Skin** Harmful if absorbed through skin. Causes skin irritation.  
**Eyes** Causes eye irritation.  
**Ingestion** Harmful if swallowed.

---

**3. COMPOSITION/INFORMATION ON INGREDIENTS**

Synonyms : 4-Allyl-1,2-methylenedioxybenzene  
5-Allyl-1,3-benzodioxole

Formula : C<sub>10</sub>H<sub>10</sub>O<sub>2</sub>  
Molecular Weight : 162.19 g/mol

CAS-No.	EC-No.	Index-No.	Concentration
<b>5-Allyl-1,3-benzodioxole</b>			
94-59-7	202-345-4	605-020-00-9	-

---

**4. FIRST AID MEASURES****General advice**

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

**If inhaled**

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**In case of skin contact**

Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**

Flush eyes with water as a precaution.

**If swallowed**

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

---

**5. FIREFIGHTING MEASURES****Conditions of flammability**

Not flammable or combustible.

**Suitable extinguishing media**

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

**Special protective equipment for firefighters**

Wear self contained breathing apparatus for fire fighting if necessary.

**Hazardous combustion products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides

**Explosion data - sensitivity to mechanical impact**

no data available

**Explosion data - sensitivity to static discharge**

no data available

---

**6. ACCIDENTAL RELEASE MEASURES****Personal precautions**

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

**Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

**Methods and materials for containment and cleaning up**

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

---

**7. HANDLING AND STORAGE****Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

**Conditions for safe storage**

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

---

**8. EXPOSURE CONTROLS/PERSONAL PROTECTION**

Contains no substances with occupational exposure limit values.

**Personal protective equipment****Respiratory protection**

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Hand protection**

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

**Eye protection**

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

**Skin and body protection**

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

**Hygiene measures**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

**Specific engineering controls**

Use mechanical exhaust or laboratory fumehood to avoid exposure.

---

**9. PHYSICAL AND CHEMICAL PROPERTIES****Appearance**

Form clear, liquid

Colour yellow

**Safety data**

pH no data available

Melting point/freezing point Melting point/range: 11.2 °C (52.2 °F) - lit.

Boiling point 232 - 234 °C (450 - 453 °F) - lit.

Flash point 100 °C (212 °F) - closed cup

Ignition temperature no data available

Autoignition no data available

temperature	
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	no data available
Density	1.095 g/mL at 25 °C (77 °F)
Water solubility	no data available
Partition coefficient: n-octanol/water	no data available
Relative vapour density	no data available
Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

---

## 10. STABILITY AND REACTIVITY

### Chemical stability

Stable under recommended storage conditions.

### Possibility of hazardous reactions

no data available

### Conditions to avoid

no data available

### Materials to avoid

Strong oxidizing agents

### Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides  
Other decomposition products - no data available

---

## 11. TOXICOLOGICAL INFORMATION

### Acute toxicity

#### Oral LD50

LD50 Oral - rat - 1,950 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity).

#### Inhalation LC50

no data available

#### Dermal LD50

LD50 Dermal - rabbit - > 5,000 mg/kg

#### Other information on acute toxicity

no data available

### Skin corrosion/irritation

Skin - rabbit - Skin irritation - 24 h

### Serious eye damage/eye irritation

no data available

### Respiratory or skin sensitization

no data available

### Germ cell mutagenicity

Laboratory experiments have shown mutagenic effects.  
In vitro tests showed mutagenic effects

### **Carcinogenicity**

This product is or contains a component that has been reported to be probably carcinogenic based on its IARC, OSHA, ACGIH, NTP, or EPA classification.

Possible human carcinogen

IARC: 2B - Group 2B: Possibly carcinogenic to humans (5-Allyl-1,3-benzodioxole)

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

### **Reproductive toxicity**

no data available

### **Teratogenicity**

no data available

### **Specific target organ toxicity - single exposure (Globally Harmonized System)**

no data available

### **Specific target organ toxicity - repeated exposure (Globally Harmonized System)**

no data available

### **Aspiration hazard**

no data available

### **Potential health effects**

<b>Inhalation</b>	May be harmful if inhaled. Causes respiratory tract irritation.
<b>Ingestion</b>	Harmful if swallowed.
<b>Skin</b>	Harmful if absorbed through skin. Causes skin irritation.
<b>Eyes</b>	Causes eye irritation.

### **Signs and Symptoms of Exposure**

Liver injury may occur., Kidney injury may occur.

### **Synergistic effects**

no data available

### **Additional Information**

RTECS: CY2800000

---

## **12. ECOLOGICAL INFORMATION**

### **Toxicity**

no data available

### **Persistence and degradability**

no data available

### **Bioaccumulative potential**

no data available

### **Mobility in soil**

no data available

**PBT and vPvB assessment**

no data available

**Other adverse effects**

no data available

---

**13. DISPOSAL CONSIDERATIONS**

**Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

**Contaminated packaging**

Dispose of as unused product.

---

**14. TRANSPORT INFORMATION**

**DOT (US)**

UN number: 3082    Class: 9    Packing group: III  
Proper shipping name: Environmentally hazardous substances, liquid, n.o.s. (5-Allyl-1,3-benzodioxole)  
Reportable Quantity (RQ): 100 lbs  
Marine pollutant: No  
Poison Inhalation Hazard: No

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

---

**15. REGULATORY INFORMATION**

**WHMIS Classification**

D2A	Very Toxic Material Causing Other Toxic Effects	Carcinogen
D2B	Toxic Material Causing Other Toxic Effects	Moderate skin irritant
		Mutagen

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all the information required by the Controlled Products Regulations.

---

**16. OTHER INFORMATION**

**Further information**

Copyright 2012 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only. The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.