

### SECTION 1: Identification of the substance/mixture and of the company/undertaking

#### 1.1. Product identifier

|                 |   |
|-----------------|---|
| Product form    | : Substance   |
| Trade name      | : Isosafrole  |
| EC no           | : 204-410-2   |
| CAS No          | : 120-58-1  |
| Product code    | : SB17111   |
| Type of product | : Isomer mixture  |
| Formula         | : C10H10O2  |
| Synonyms        | : 1,2-(methylenedioxy)-4-propenylbenzene / 1,2-(methylenedioxy)-4-propenylbenzene, mixture of cis and trans / 1,2-methylenedioxy-4-propenylbenzene / 1,2-methylenedioxy-4-propenylbenzene, mixture of cis and trans isomers / 1,3-benzodioxole, 5-(1-propenyl)- / 3,4-(methylenedioxy)propenylbenzene / 3,4-methylenedioxy-1-propenyl benzene / 4-propenyl-1,2-methylenedioxybenzene / 4-propenylcatechol methylene ether / 5-(1-propenyl)-1,3-benzodioxole / 5-(propen-1-yl)-1,3-benzodioxole / 6-(1-propenyl)-1,3-benzodioxole / benzene, 1,2-(methylenedioxy)-4-propenyl- / isosafrol / isosafrol (cis+trans) / isosafrol, mixture of cis and trans / isosafrole |
| BIG no          | : 29284   |

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

##### 1.2.1. Relevant identified uses

|                              |   |
|------------------------------|---|
| Main use category            | : Professional use, Industrial use                |
| Use of the substance/mixture | : Certified reference material for laboratory use |
| Function or use category     | : Laboratory chemicals                            |

##### 1.2.2. Uses advised against

No additional information available

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

##### Spectracer UK Ltd.

Second Floor,  
27 Gloucester Place,  
London,  
W1U 8HU,  
United Kingdom.

Tel: +44 (0) 207 193 9114

Fax: +44 (0) 203 432 4686

Email: [contact@spectracer.co.uk](mailto:contact@spectracer.co.uk)

Web: [www.spectracer.com](http://www.spectracer.com)

#### 1.4. Emergency telephone number

Emergency number : Tel: +44(0)1933 445260 Option 1. Language: English only.  
For Chemical Emergencies Only  
Llewellyn (Safety Advisors) Europe Ltd

| Country        | Organisation/Company                                     | Address   | Emergency number  | Comment |
|----------------|--|---|---|---------|
| Ireland        | National Poisons Information Centre<br>Beaumont Hospital | Beaumont Hospital Beaumont Road<br>9 Dublin           | : +353 1 8379964  |         |
| United Kingdom | National Poisons Information Service (NHS Direct)        | <a href="http://www.npis.org">http://www.npis.org</a> | 111 (England & Wales only) or 112 (EU) or 08454 24 24 24 (Scotland) |         |

### SECTION 2: Hazards identification

#### 2.1. Classification of the substance or mixture

##### Classification according to Regulation (EC) No. 1272/2008 [CLP]

Acute toxicity (oral), H302  
Category 4

Full text of hazard classes and H-statements : see section 16

### Adverse physicochemical, human health and environmental effects

Harmful if swallowed.

### 2.2. Label elements

#### Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS07

Signal word (CLP) :

Warning

Hazard statements (CLP) :

H302 - Harmful if swallowed

Precautionary statements (CLP) :

P264 - Wash hands and other exposed areas thoroughly after handling  
 P270 - Do not eat, drink or smoke when using this product  
 P301+P312 - IF SWALLOWED: Call a POISON CENTER or doctor if you feel unwell  
 P330 - Rinse mouth  
 P501 - Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation

### 2.3. Other hazards

No additional information available

## SECTION 3: Composition/information on ingredients

### 3.1. Substance

| Name  | Product identifier                     | %     | Classification according to Regulation (EC) No. 1272/2008 [CLP] |
|---|--|-------|---|
| isosafrole,mixture of isomers cis and trans | (CAS No) 120-58-1<br>(EC no) 204-410-2 | >= 95 | Acute Tox. 4 (Oral), H302                                       |

Full text of H-statements: see section 16

### 3.2. Mixture

Not applicable

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

|                                       |   |
|---------------------------------------|---|
| First-aid measures general            | : Check the vital functions. Unconscious: maintain adequate airway and respiration. Respiratory arrest: artificial respiration or oxygen. Cardiac arrest: perform resuscitation. Victim conscious with laboured breathing: half-seated. Victim in shock: on his back with legs slightly raised. Vomiting: prevent asphyxia/aspiration pneumonia. Prevent cooling by covering the victim (no warming up). Keep watching the victim. Give psychological aid. Keep the victim calm, avoid physical strain. Depending on the victim's condition: doctor/hospital. |
| First-aid measures after inhalation   | : Remove the victim into fresh air.   |
| First-aid measures after skin contact | : Wash immediately with lots of water (15 minutes)/shower. Remove clothing while washing.   |
| First-aid measures after eye contact  | : Rinse immediately with plenty of water for 15 minutes. Take victim to an ophthalmologist. Do not apply neutralizing agents.   |
| First-aid measures after ingestion    | : Rinse mouth with water. Ingestion of large quantities: immediately to hospital. Call Poison Information Centre.   |

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

Symptoms/injuries after skin contact : ON CONTINUOUS EXPOSURE/CONTACT: Tingling/irritation of the skin.

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

Treat symptomatically.

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

|                                |  |
|--------------------------------|--|
| Suitable extinguishing media   | : Water spray. Polyvalent foam. BC-powder. Carbon dioxide. |
| Unsuitable extinguishing media | : No unsuitable extinguishing media known.                 |

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

|  |   |
|--|---|
| Fire hazard                                      | : DIRECT FIRE HAZARD: Insufficient data available on direct fire hazard (flashpoint > 100°C).   |
| Explosion hazard                                 | : DIRECT EXPLOSION HAZARD: No data available on direct explosion hazard. INDIRECT EXPLOSION HAZARD: No data available on indirect explosion hazard. |
| Hazardous decomposition products in case of fire | : Toxic fumes may be released.  |

### 5.3. Advice for firefighters

|                                |   |
|--------------------------------|---|
| Precautionary measures fire    | : Exposure to fire/heat: keep upwind. Exposure to fire/heat: have neighbourhood close doors and windows.                    |
| Firefighting instructions      | : Take account of environmentally hazardous firefighting water. Use water moderately and if possible collect or contain it. |
| Protection during firefighting | : Heat/fire exposure: compressed air/oxygen apparatus.  |

## SECTION 6: Accidental release measures

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

#### 6.1.1. For non-emergency personnel

|                      |  |
|----------------------|--|
| Protective equipment | : Gloves. Face-shield. Protective clothing. See "Material-Handling" to select protective clothing. |
| Emergency procedures | : Mark the danger area. Wash contaminated clothes.   |

#### 6.1.2. For emergency responders

|                      |   |
|----------------------|---|
| Protective equipment | : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection". |
|----------------------|---|

### 6.2. Environmental precautions

Prevent soil and water pollution. Prevent spreading in sewers.

### 6.3. Methods and material for containment and cleaning up

|                         |  |
|-------------------------|--|
| For containment         | : Contain released substance, pump into suitable containers. Plug the leak, cut off the supply. Dam up the liquid spill.   |
| Methods for cleaning up | : Take up liquid spill into absorbent material, e.g.: slaked lime or soda ash. Scoop absorbed substance into closing containers. Carefully collect the spill/leftovers. Clean contaminated surfaces with an excess of water. Wash clothing and equipment after handling. |
| Other information       | : Dispose of materials or solid residues at an authorized site.  |

### 6.4. Reference to other sections

For further information refer to section 13.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

|                               |   |
|-------------------------------|---|
| Precautions for safe handling | : Comply with the legal requirements. Clean contaminated clothing. Do not discharge the waste into the drain. Observe normal hygiene standards. Keep container tight closed. Carry out operations in the open/under local exhaust/ventilation or with respiratory protection. |
| Hygiene measures              | : Do not eat, drink or smoke when using this product. Always wash hands after handling the product.   |

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

|                               |  |
|-------------------------------|--|
| Storage conditions            | : Store in a well-ventilated place. Keep cool.   |
| Heat and ignition sources     | : KEEP SUBSTANCE AWAY FROM: heat sources.  |
| Prohibitions on mixed storage | : KEEP SUBSTANCE AWAY FROM: oxidizing agents.  |
| Storage area                  | : Meet the legal requirements.   |
| Special rules on packaging    | : SPECIAL REQUIREMENTS: closing. correctly labelled. meet the legal requirements. Secure fragile packagings in solid containers. |
| Packaging materials           | : Suitable packing materials. glass.   |

### 7.3. Specific end use(s)

No additional information available

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

No additional information available

### 8.2. Exposure controls

|                                   |   |
|-----------------------------------|---|
| Appropriate engineering controls  | : Ensure good ventilation of the work station.                              |
| Personal protective equipment     | : Avoid all unnecessary exposure. Gloves. Protective clothing. Face shield. |
| Materials for protective clothing | : GIVE GOOD RESISTANCE: rubber. plastics                                    |
| Hand protection                   | : Gloves  |
| Eye protection                    | : Face-shield   |
| Skin and body protection          | : Protective clothing   |
| Respiratory protection            | : On heating: Gas mask  |



Environmental exposure controls : Avoid release to the environment.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

|  |   |
|--|---|
| Physical state                             | : Liquid  |
| Appearance                                 | : Liquid.   |
| Molecular mass                             | : 162,19 g/mol  |
| Colour                                     | : Colourless to yellow.                                     |
| Odour                                      | : Characteristic odour.                                     |
| Odour threshold                            | : No data available   |
| pH   | : No data available   |
| Relative evaporation rate (butylacetate=1) | : No data available   |
| Melting point                              | : 8 °C  |
| Freezing point                             | : No data available   |
| Boiling point                              | : 253 °C  |
| Flash point                                | : > 110 °C  |
| Auto-ignition temperature                  | : No data available   |
| Decomposition temperature                  | : No data available   |
| Flammability (solid, gas)                  | : Not applicable  |
| Vapour pressure                            | : No data available   |
| Relative vapour density at 20 °C           | : No data available   |
| Relative density                           | : 1,1   |
| Density                                    | : 1114 kg/m <sup>3</sup>                                    |
| Solubility                                 | : Insoluble in water. Soluble in ethanol. Soluble in ether. |
| Log Pow                                    | : No data available   |
| Viscosity, kinematic                       | : No data available   |
| Viscosity, dynamic                         | : No data available   |
| Explosive properties                       | : No data available   |
| Oxidising properties                       | : No data available   |
| Explosive limits                           | : No data available   |

### 9.2. Other information

Other properties : Gas/vapour heavier than air at 20°C. Slightly volatile.

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

On heating/burning: release of carbon monoxide - carbon dioxide.

### 10.2. Chemical stability

No data available.

### 10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

### 10.4. Conditions to avoid

None under recommended storage and handling conditions (see section 7).

### 10.5. Incompatible materials

No additional information available

### 10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity : Oral: Harmful if swallowed.

| Isosafrole (120-58-1)                              |                  |
|--|------------------|
| LD50 oral rat                                      | 1340 mg/kg (Rat) |
| Skin corrosion/irritation                          | : Not classified |
| Serious eye damage/irritation                      | : Not classified |
| Respiratory or skin sensitisation                  | : Not classified |
| Germ cell mutagenicity                             | : Not classified |
| Carcinogenicity                                    | : Not classified |
| Reproductive toxicity                              | : Not classified |
| Specific target organ toxicity (single exposure)   | : Not classified |
| Specific target organ toxicity (repeated exposure) | : Not classified |
| Aspiration hazard                                  | : Not classified |
| IARC group   | : 3              |

## SECTION 12: Ecological information

### 12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms nor to cause long-term adverse effects in the environment.  
 Ecology - water : water pollutant (surface water). No data available on ecotoxicity.

### 12.2. Persistence and degradability

| Isosafrole (120-58-1)         |   |
|-------------------------------|---|
| Persistence and degradability | Biodegradability in water: no data available. |

### 12.3. Bioaccumulative potential

| Isosafrole (120-58-1)     |                                     |
|---------------------------|-------------------------------------|
| Bioaccumulative potential | Bioaccumulation: No data available. |

### 12.4. Mobility in soil

No additional information available

### 12.5. Results of PBT and vPvB assessment

No additional information available

### 12.6. Other adverse effects

No additional information available

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

Waste treatment methods : Dispose of contents/container in accordance with licensed collector's sorting instructions.  
 Waste disposal recommendations : Remove waste in accordance with local and/or national regulations. Hazardous waste shall not be mixed together with other waste. Different types of hazardous waste shall not be mixed together if this may entail a risk of pollution or create problems for the further management of the waste. Hazardous waste shall be managed responsibly. All entities that store, transport or handle hazardous waste shall take the necessary measures to prevent risks of pollution or damage to people or animals. Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber with energy recovery.  
 Additional information : Hazardous waste according to Directive 2008/98/EC.

### SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

| ADR                                     | IMDG          | IATA          | ADN           | RID           |
|---|---------------|---------------|---------------|---------------|
| <b>14.1. UN number</b>                  |               |               |               |               |
| Not regulated                           | Not regulated | Not regulated | Not regulated | Not regulated |
| <b>14.2. UN proper shipping name</b>    |               |               |               |               |
| Not regulated                           | Not regulated | Not regulated | Not regulated | Not regulated |
| Not regulated                           | Not regulated | Not regulated | Not regulated | Not regulated |
| <b>14.3. Transport hazard class(es)</b> |               |               |               |               |
| Not regulated                           | Not regulated | Not regulated | Not regulated | Not regulated |
| Not regulated                           | Not regulated | Not regulated | Not regulated | Not regulated |
| <b>14.4. Packing group</b>              |               |               |               |               |
| Not regulated                           | Not regulated | Not regulated | Not regulated | Not regulated |
| <b>14.5. Environmental hazards</b>      |               |               |               |               |
| Not regulated                           | Not regulated | Not regulated | Not regulated | Not regulated |
| No supplementary information available  |               |               |               |               |

#### 14.6. Special precautions for user

##### - Overland transport

Not regulated

##### - Transport by sea

Not regulated

##### - Air transport

Not regulated

##### - Inland waterway transport

Not regulated

##### - Rail transport

Not regulated

#### 14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

### SECTION 15: Regulatory information

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

##### 15.1.1. EU-Regulations

The following restrictions are applicable according to Annex XVII of the REACH Regulation (EC) No 1907/2006:

|  |            |
|--|------------|
| 3. Liquid substances or mixtures which are regarded as dangerous in accordance with Directive 1999/45/EC or are fulfilling the criteria for any of the following hazard classes or categories set out in Annex I to Regulation (EC) No 1272/2008 | Isosafrole |
|--|------------|

Isosafrole is not on the REACH Candidate List

Isosafrole is not on the REACH Annex XIV List

##### 15.1.2. National regulations

###### Germany

- VwVwS Annex reference : Water hazard class (WGK) 2, hazard to waters  
 WGK remark : Internal classification water polluting based on standard worst-case evaluation points due to insufficient data  
 12th Ordinance Implementing the Federal Immission Control Act - 12.BImSchV : Is not subject of the 12. BImSchV (Hazardous Incident Ordinance)

###### Netherlands

- SZW-lijst van kankerverwekkende stoffen : The substance is not listed  
 SZW-lijst van mutagene stoffen : The substance is not listed

NIET-limitatieve lijst van voor de voortplanting  
giftige stoffen – Borstvoeding : The substance is not listed

NIET-limitatieve lijst van voor de voortplanting  
giftige stoffen – Vruchtbaarheid : The substance is not listed

NIET-limitatieve lijst van voor de voortplanting  
giftige stoffen – Ontwikkeling : The substance is not listed

### Denmark

Recommendations Danish Regulation : Young people below the age of 18 years are not allowed to use the product

### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out

## SECTION 16: Other information

Full text of H- and EUH-statements:

|                     |                                   |
|---------------------|-----------------------------------|
| Acute Tox. 4 (Oral) | Acute toxicity (oral), Category 4 |
| H302                | Harmful if swallowed              |

SDS EU Mod H F (REACH ANNEX II)

*This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.*