

## SAFETY DATA SHEET

Version 5.0  
Revision Date 11/19/2014  
Print Date 11/05/2018

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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : Ligustilide

Product Number : SMB00400  
Brand : Sigma

CAS-No. : 4431-01-0

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

Identified uses : Laboratory chemicals, Manufacture of substances

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

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

## 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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2. HAZARDS IDENTIFICATION

## 2.1 Classification of the substance or mixture

**GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Acute toxicity, Oral (Category 3), H301

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word : Danger

Hazard statement(s)  
H301 : Toxic if swallowed.

Precautionary statement(s)  
P264 : Wash skin thoroughly after handling.  
P270 : Do not eat, drink or smoke when using this product.  
P301 + P310 + P330 : IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. Rinse mouth.  
P405 : Store locked up.  
P501 : Dispose of contents/ container to an approved waste disposal plant.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

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3. COMPOSITION/INFORMATION ON INGREDIENTS

## 3.1 Substances

Synonyms : 3-butylidene-4,5-dihydro-1(3H)-isobenzofuranone

Sigma - SMB00400

### 3-butylidene-4,5-dihydrophthalide

Formula : C<sub>12</sub>H<sub>14</sub>O<sub>2</sub>  
Molecular weight : 190.24 g/mol  
CAS-No. : 4431-01-0

#### Hazardous components

Component	Classification	Concentration
<b>3-butylidene-4,5-dihydro-1(3H)-isobenzofuranone</b>		
	Acute Tox. 3; H301	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

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## 4. FIRST AID MEASURES

### 4.1 Description of 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. Take victim immediately to hospital. 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.

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data available

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## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

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

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

Carbon oxides

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

No data available

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## 6. ACCIDENTAL RELEASE MEASURES

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

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

### 6.2 Environmental precautions

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

### 6.3 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.

### 6.4 Reference to other sections

For disposal see section 13.

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## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.  
For precautions see section 2.2.

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

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.

Recommended storage temperature -20 °C

Air and light sensitive.

Storage class (TRGS 510): Non-combustible, acute toxic Cat.3 / toxic hazardous materials or hazardous materials causing chronic effects

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

#### Personal protective equipment

##### Eye/face 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 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.

##### 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.

##### 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).

##### Control of environmental exposure

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

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |                                 |                                |
|---------------------------------|--------------------------------|
| a) Appearance                   | Form: liquid<br>Colour: yellow |
| b) Odour                        | No data available              |
| c) Odour Threshold              | No data available              |
| d) pH                           | No data available              |
| e) Melting point/freezing point | No data available              |

f)	Initial boiling point and boiling range	No data available
g)	Flash point	No data available
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapour pressure	No data available
l)	Vapour density	No data available
m)	Relative density	1.1 g/cm <sup>3</sup>
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	log Pow: 2.574
p)	Auto-ignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

## 9.2 Other safety information

No data available

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

Other decomposition products - No data available  
In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

No data available

**Skin corrosion/irritation**

No data available

**Serious eye damage/eye irritation**

No data available

**Respiratory or skin sensitisation**

No data available

**Germ cell mutagenicity**

No data available

**Carcinogenicity**

- IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
- 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.
- NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
- OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**

No data available

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: NP6810000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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**12. ECOLOGICAL INFORMATION****12.1 Toxicity**

No data available

**12.2 Persistence and degradability**

No data available

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**12.6 Other adverse effects**

No data available

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

#### 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.

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## 14. TRANSPORT INFORMATION

### DOT (US)

UN number: 2810      Class: 6.1      Packing group: III  
Proper shipping name: Toxic, liquids, organic, n.o.s. (3-butylidene-4,5-dihydro-1(3H)-isobenzofuranone)  
Reportable Quantity (RQ):

Poison Inhalation Hazard: No

### IMDG

UN number: 2810      Class: 6.1      Packing group: III      EMS-No: F-A, S-A  
Proper shipping name: TOXIC LIQUID, ORGANIC, N.O.S. (3-butylidene-4,5-dihydro-1(3H)-isobenzofuranone)

### IATA

UN number: 2810      Class: 6.1      Packing group: III  
Proper shipping name: Toxic liquid, organic, n.o.s. (3-butylidene-4,5-dihydro-1(3H)-isobenzofuranone)

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## 15. REGULATORY INFORMATION

### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### SARA 311/312 Hazards

Acute Health Hazard

### Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
3-butylidene-4,5-dihydro-1(3H)-isobenzofuranone	4431-01-0	

### New Jersey Right To Know Components

	CAS-No.	Revision Date
3-butylidene-4,5-dihydro-1(3H)-isobenzofuranone	4431-01-0	

### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## 16. OTHER INFORMATION

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

Acute Tox. H301	Acute toxicity Toxic if swallowed.
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**HMIS Rating**

Health hazard:	2
Chronic Health Hazard:	
Flammability:	0
Physical Hazard	0

**NFPA Rating**

Health hazard:	2
Fire Hazard:	0
Reactivity Hazard:	0

**Further information**

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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.

**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

Version: 5.0

Revision Date: 11/19/2014

Print Date: 11/05/2018