SAFETY DATA SHEET

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

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, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO  63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 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) : Toxic if swallowed.
Precautionary statement(s) : 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/ doctor. 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

SECTION 3: Composition/information on ingredients

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

Formula : C12H14O2
Molecular weight : 190.24 g/mol
CAS-No. : 4431-01-0

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-butylidene-4,5-dihydro-1(3H)-isobenzofuranone</td>
<td>Acute Tox. 3; H301</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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

SECTION 4: First aid measures

4.1  Description of first-aid measures

General advice
Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact
After eye contact: rinse out with plenty of water. Remove contact lenses.

If swallowed
If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

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
SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Water Foam Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Combustible.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information
Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.
For personal protection see section 8.

6.2 Environmental precautions
Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability
Recommended storage temperature
-20 °C
Air and light sensitive.

**Storage class**
Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which 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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**SECTION 8: Exposure controls/personal protection**

**8.1 Control parameters**

**Ingredients with workplace control parameters**
Contains no substances with occupational exposure limit values.

**8.2 Exposure controls**

**Appropriate engineering controls**
Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

**Personal protective equipment**

**Eye/face protection**
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

**Skin protection**
required

**Body Protection**
protective clothing

**Respiratory protection**
required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

**Control of environmental exposure**
Do not let product enter drains.

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**SECTION 9: Physical and chemical properties**

**9.1 Information on basic physical and chemical properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Appearance</strong></td>
<td>Form: liquid</td>
</tr>
<tr>
<td></td>
<td>Color: yellow</td>
</tr>
<tr>
<td><strong>Odor</strong></td>
<td>No data available</td>
</tr>
<tr>
<td><strong>Odor Threshold</strong></td>
<td>No data available</td>
</tr>
<tr>
<td><strong>pH</strong></td>
<td>No data available</td>
</tr>
<tr>
<td><strong>Melting point/freezing point</strong></td>
<td>No data available</td>
</tr>
<tr>
<td><strong>Initial boiling point</strong></td>
<td>No data available</td>
</tr>
</tbody>
</table>
and boiling range

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) Vapor pressure No data available

l) Vapor density No data available

m) Density 1.1 g/cm³

Relative density No data available

n) Water solubility No data available

o) Partition coefficient: n-octanol/water log Pow: 2.574

p) Autoignition temperature No data available

q) Decomposition temperature No data available

r) Viscosity No data available

s) Explosive properties No data available

t) Oxidizing properties none

9.2 Other safety information
No data available

SECTION 10: Stability and reactivity

10.1 Reactivity
No data available

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
no information available

10.5 Incompatible materials
Strong oxidizing agents

10.6 Hazardous decomposition products
In the event of fire: see section 5
SECTION 11: Toxicological information

11.1 Information on toxicological effects

**Acute toxicity**
- Oral: No data available
- Inhalation: No data available
- Dermal: No data available

**Skin corrosion/irritation**
- No data available

**Serious eye damage/eye irritation**
- No data available

**Respiratory or skin sensitization**
- No data available

**Germ cell mutagenicity**
- No data available

**Carcinogenicity**
- IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
- NTP: No ingredient 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 on OSHA’s list of regulated carcinogens.

**Reproductive toxicity**
- 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

11.2 Additional Information

RTECS: NP6810000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 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 Endocrine disrupting properties
No data available

12.7 Other adverse effects
No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

**Product**
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 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)
IATA Passenger: Not permitted for transport
IATA Cargo: Not permitted for transport

SECTION 15: Regulatory information

**SARA 302 Components**
This material does not contain any components with a section 302 EHS TPQ.

**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.

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**SECTION 16: Other information**

**Further information**
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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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