

# Isoimperatorin SDS/MSDS (Safety Data Sheet)

## 1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

\* Product Name: Isoimperatorin

\* Catalog Number: S3904

\* CAS Number: 482-45-1

\* IUPAC Name: 7H-Furo[3,2-g][1]benzopyran-7-one, 4-[(3-methyl-2-buten-1-yl)oxy]-

Relevant identified uses and uses advised against

\* Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.

\* Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

\* Company: Selleck Chemicals

\* TollFree: +1 877 796-6397

\* Tel: +1 832 582-8158

\* Fax: +1 832 582-8590

Emergency telephone number

\* Emergency phone #: +1 832 582-8158

## 2. HAZARDS IDENTIFICATION

### 2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

Acute toxicity (oral): Category 4. H302

Skin irritation: Category 2. H315

Skin sensitization: Category 1. H317

Serious eye irritation: Category 2. H319

Specific target organ toxicity (single exposure): Category 3. H335

### 2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Warning

Hazard statement(s)

H302: Harmful if swallowed  
H315: Causes skin irritation  
H317: May cause an allergic skin reaction  
H319: Causes serious eye irritation  
H335: May cause respiratory irritation

Precautionary statement(s)

None.

|                   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|-------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Prevention</b> | <p>P261: Avoid breathing dust/fume/gas/mist/vapors/spray.</p> <p>P264: Wash hands thoroughly after handling.</p> <p>P264+P265: Wash hands thoroughly after handling. Do not touch eyes.</p> <p>P270: Do not eat, drink or smoke when using this product.</p> <p>P271: Use only outdoors or in a well-ventilated area.</p> <p>P272: Contaminated work clothing should not be allowed out of the workplace.</p> <p>P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.</p>                                                                                                                                                                                                                                                                                                    |
| <b>Response</b>   | <p>P301+P317: IF SWALLOWED: Get medical help.</p> <p>P302+P352: IF ON SKIN: wash with plenty of water.</p> <p>P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing.</p> <p>P305+P351: IF IN EYES: Rinse cautiously with water for several minutes.</p> <p>P319: Get medical help if you feel unwell.</p> <p>P321: Specific treatment (see information on this label and safety datasheet)).</p> <p>P330: Rinse mouth.</p> <p>P332+P317: If skin irritation occurs: Get medical help.</p> <p>P333+P317: If skin irritation or rash occurs: Get medical help.</p> <p>P337+P317: If eye irritation persists: Get medical help.</p> <p>P338: Remove contact lenses, if present and easy to do. Continue rinsing.</p> <p>P362+P364: Take off contaminated clothing and wash it before reuse.</p> |
| <b>Storage</b>    | <p>P403+P233: Store in a well-ventilated place. Keep container tightly closed.</p> <p>P405: Store locked up.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| <b>Disposal</b>   | <p>P501: P501 Dispose of contents/ container to an approved waste disposal plant.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |

### 2.3 Other hazards

None.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Product name: Isoimperatorin  
CAS Number: 482-45-1  
PubChem CID: 68081  
Molecular formula: C<sub>16</sub>H<sub>14</sub>O<sub>4</sub>  
Molecular weight: 270.28 g/mol  
IUPAC name: 4-(3-methylbut-2-enoxy)furo[3,2-g]chromen-7-one

### 3.2 Mixtures

Not applicable (pure substance).

## 4. FIRST-AID MEASURES

### 4.1 Description of first aid measures

Inhalation: Move to fresh air. Keep at rest in a position comfortable for breathing. Seek medical attention if symptoms persist.

Skin contact: Wash with plenty of soap and water. Remove contaminated clothing. Seek medical attention if irritation develops.

Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention.

Ingestion: Rinse mouth. Do NOT induce vomiting unless directed by medical personnel. Seek medical attention.

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

See Section 11 (Toxicological Information).

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

Treat symptomatically. Contact a poison control center or physician for severe exposure.

### **5. FIRE-FIGHTING MEASURES**

#### **5.1 Extinguishing media**

Suitable: Water spray, dry chemical, carbon dioxide (CO<sub>2</sub>), alcohol-resistant foam.

Unsuitable: None known.

#### **5.2 Specific hazards arising from the substance or mixture**

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Advice for firefighters: Wear self-contained breathing apparatus for firefighting if necessary.

#### **5.3 Advice for firefighters**

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

### **6. ACCIDENTAL RELEASE MEASURES**

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

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

#### **6.2 Environmental precautions**

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

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

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Avoid dust formation. Avoid breathing vapors, mist or gas. Environmental precautions: Do not let product enter drains. Methods and materials for containment and cleaning up: Sweep up and shovel. Keep in suitable, closed containers for disposal.

SRP: Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in air, soil or water; effects on animal, aquatic and plant life; and conformance with environmental and public health regulations. If it is possible or reasonable use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination.

Product: Offer surplus and non-recyclable solutions to a licensed disposal company. Contaminated packaging: Dispose of as unused product.

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Avoid dust formation. Avoid breathing vapors, mist or gas. Environmental precautions: Do not let product enter drains.

Precautions for safe handling: Provide appropriate exhaust ventilation at places where dust is formed.

Appropriate engineering controls: General industrial hygiene practice.

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.

SRP: Local exhaust ventilation should be applied wherever there is an incidence of point source emissions or dispersion of regulated contaminants in the work area. Ventilation control of the contaminant as close to its point of generation is both the most economical and safest method to minimize personnel exposure to airborne contaminants. Ensure that the local ventilation moves the contaminant away from the worker.

## **7. HANDLING AND STORAGE**

### **7.1 Precautions for safe handling**

Keep container tightly closed in a dry and well-ventilated place. Recommended storage temperature: 2-8 °C. Keep in a dry place. Store in the dark.

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

Keep container tightly closed in a dry and well-ventilated place. Recommended storage temperature: 2-8 °C. Keep in a dry place. Store in the dark.

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

## **8. EXPOSURE CONTROLS/PERSONAL PROTECTION**

### **8.1 Exposure controls**

#### **8.1.1 Occupational exposure limits (OEL)**

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

#### **8.1.2 Appropriate engineering controls**

Use only in a chemical fume hood or with local exhaust ventilation.

Ensure adequate ventilation to keep airborne concentrations below exposure limits.

### **8.2 Individual protection measures**

#### **8.2.1 Eye/face protection**

Wear chemical safety goggles.

#### **8.2.2 Skin protection**

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

#### 8.2.3 Respiratory protection

Use NIOSH-approved dust/mist respirator (N95 or higher) if ventilation is inadequate.

#### 8.2.4 Thermal hazards

Not applicable.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- a) Appearance: Off-white, light brown solid
- b) Odor: No data available
- c) Odor threshold: No data available
- d) pH: No data available
- e) Melting point/freezing point: 98-100 °C
- 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) Vapor pressure: No data available
- l) Vapor density: No data available
- m) Relative density: No data available
- n) Water solubility: Soluble in DMSO; slightly soluble in water
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 3.8
- 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 information

Topological Polar Surface Area (TPSA): 48.7 Å<sup>2</sup>

Complexity: 436

## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

#### 10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

#### 10.5 Incompatible materials

Incompatible materials: Strong oxidizing agents.

#### 10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

See also Section 5 (Fire-fighting measures) for combustion products.

### 11. TOXICOLOGICAL INFORMATION

#### 11.1 Information on toxicological effects

##### Acute toxicity:

No acute toxicity data available.

##### Skin corrosion/irritation:

Causes skin irritation (H315).

##### Serious eye damage/eye irritation:

Causes serious eye irritation (H319).

##### Respiratory or skin sensitization:

May cause an allergic skin reaction (H317).

##### Germ cell mutagenicity:

No data available.

##### Carcinogenicity:

No data available.

##### 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

##### Carcinogen classification:

Not listed by IARC. IARC has assessed other furocoumarins, classifying 8-methoxypsoralen as carcinogenic to humans (Group 1), 5-methoxypsoralen as possibly carcinogenic to humans (Group 2A), and certain other furocoumarins as not being classifiable as to their carcinogenicity to humans (Group 3). (L135)

##### Signs and symptoms of exposure:

Symptoms of low dose exposure include excessive salivation and eye-watering. Acute dose symptoms include severe nausea/vomiting, salivation, sweating, bradycardia, hypotension, collapse, and convulsions. Increasing muscle weakness is a possibility and may result in death if respiratory muscles are involved. Hypertension, hypoglycemia, anxiety, headache, tremor and ataxia may also result.

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

## **12. ECOLOGICAL INFORMATION**

### **12.1 Toxicity**

Isoimperatorin's production and use as a laboratory chemical and in the manufacture of substances may result in its release to the environment through various waste streams. Isoimperatorin has been detected in various plants. If released to air, an estimated vapor pressure of  $1.4 \times 10^{-7}$  mm Hg at 25 °C indicates isoimperatorin will exist in both the vapor and particulate phases in the atmosphere. Vapor-phase isoimperatorin will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 2 hours. Particulate-phase isoimperatorin will be removed from the atmosphere by wet and dry deposition. Isoimperatorin has a light absorption peak at 310 nm and, therefore, may be susceptible to direct photolysis by sunlight. If released to soil, isoimperatorin is expected to have slight mobility based upon an estimated Koc of 4500. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of  $2.0 \times 10^{-10}$  atm-cu m/mole. Isoimperatorin is not expected to volatilize from dry soil surfaces based upon its estimated vapor pressure. Biodegradation data in soil and water were not available. If released into water, isoimperatorin is expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law c

### **12.2 Persistence and degradability**

No data available.

### **12.3 Bioaccumulative potential**

Log P (n-octanol/water): 3.8

Potential for bioaccumulation exists (Log P > 3).

### **12.4 Mobility in soil**

No data available.

### **12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available.

### **12.6 Other adverse effects**

No other adverse ecological effects identified.

## **13. DISPOSAL CONSIDERATIONS**

### **13.1 Waste treatment methods**

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

## **14. TRANSPORT INFORMATION**

### **14.1 UN number**

Not regulated as dangerous goods (research quantities typically exempt).

### **14.2 UN proper shipping name**

Not subject to transport regulations (small quantities for research use).

#### **14.3 Transport hazard class(es)**

Not classified as dangerous goods for transport (research quantities).

#### **14.4 Packing group**

Not applicable (not regulated as dangerous goods in typical research quantities).

#### **14.5 Environmental hazards**

Marine pollutant: No (not classified as environmentally hazardous per GHS).

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

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

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

Not applicable.

### **15. REGULATORY INFORMATION**

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

US EPA / TSCA: Not available in public databases.

EU ECHA / REACH: Not available in public databases.

##### **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 (short-term) health hazard

##### **Massachusetts Right To Know Components:**

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

##### **Pennsylvania Right To Know Components:**

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

##### **New Jersey Right To Know Components:**

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

##### **California Prop. 65 Components:**

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

#### **15.2 Chemical safety assessment**

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

## **16. OTHER INFORMATION**

Revision Date: 2026/09/09

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product.

Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.