

## SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product identifier

Product Description: **n-Butylidenephthalide, (E)+(Z)**  
Cat No. : **A10353**  
CAS No 551-08-6  
Molecular Formula C12 H12 O2

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

Recommended Use Laboratory chemicals.  
Uses advised against No Information available

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

#### Company

Thermo Fisher (Kandel) GmbH  
Erlenbachweg 2, 76870 Kandel, Germany  
Tel: +49 (0) 721 84007 280  
Fax: +49 (0) 721 84007 300

**Swiss distributor - Fisher Scientific AG**  
Neuhofstrasse 11, CH 4153 Reinach  
Tel: +41 (0) 56 618 41 11  
<https://www.fishersci.ch/ch/en/customer-help-support/forms/email-us.html>

#### E-mail address

[begel.sdsdesk@thermofisher.com](mailto:begel.sdsdesk@thermofisher.com)

### 1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

customers in Switzerland:  
Tox Info Suisse Emergency Number: **145 (24hr)**  
Tox Info Suisse: +41-44 251 51 51 (Emergency number from abroad)  
Chemtrec (24h) Toll-Free: 0800 564 402  
Chemtrec Local: +41-43 508 20 11 (Zurich)

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

CLP Classification - Regulation (EC) No 1272/2008

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## Physical hazards

Based on available data, the classification criteria are not met

## Health hazards

Acute oral toxicity

Category 4 (H302)

## Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## 2.2. Label elements



Signal Word

Warning

## Hazard Statements

H302 - Harmful if swallowed

## Precautionary Statements

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting

P312 - Call a POISON CENTER or doctor if you feel unwell

P264 - Wash face, hands and any exposed skin thoroughly after handling

## 2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

| Component                             | CAS No   | EC No             | Weight % | CLP Classification - Regulation (EC) No 1272/2008 |
|---------------------------------------|----------|-------------------|----------|---|
| 1(3H)-Isobenzofuranone, 3-butyldiene- | 551-08-6 | EEC No. 208-991-3 | <=100    | Acute Tox. 4 (H302)                               |

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

General Advice

If symptoms persist, call a physician.

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|   |   |
|---|---|
| <b>Eye Contact</b>                        | Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.   |
| <b>Skin Contact</b>                       | Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician. |
| <b>Ingestion</b>                          | Clean mouth with water and drink afterwards plenty of water.  |
| <b>Inhalation</b>                         | Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.      |
| <b>Self-Protection of the First Aider</b> | No special precautions required.  |

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

None reasonably foreseeable.

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

**Notes to Physician** Treat symptomatically.

## **SECTION 5: FIREFIGHTING MEASURES**

### **5.1. Extinguishing media**

#### **Suitable Extinguishing Media**

Carbon dioxide (CO<sub>2</sub>). Powder. Water spray. In case of major fire and large quantities: Evacuate area. Fight fire remotely due to the risk of explosion.

#### **Extinguishing media which must not be used for safety reasons**

No information available.

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

Thermal decomposition can lead to release of irritating gases and vapors.

#### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

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

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

## **SECTION 6: ACCIDENTAL RELEASE MEASURES**

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

Ensure adequate ventilation. Use personal protective equipment as required.

### **6.2. Environmental precautions**

Should not be released into the environment. See Section 12 for additional Ecological Information.

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

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal.

### **6.4. Reference to other sections**

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Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid ingestion and inhalation. Do not get in eyes, on skin, or on clothing.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

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

Keep container tightly closed in a dry and well-ventilated place.

#### **Technical Rules for Hazardous Substances (TRGS) 510 Storage Class (LGK) (Germany)**

Storage Class/LGK 10

#### **Switzerland - Storage of hazardous substances**

<https://www.kvu.ch/de/themen/stoffe-und-produkte>  
<https://www.kvu.ch/fr/themes/substances-et-produits>  
<https://www.kvu.ch/it/temi/sostanze-e-prodotti> Storage class - SC 10/12

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

#### **Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS70 General methods for sampling airborne gases and vapours

MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

**Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)**

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No information available

## Predicted No Effect Concentration (PNEC)

No information available.

## 8.2. Exposure controls

### Engineering Measures

None under normal use conditions.

### Personal protective equipment

#### Eye Protection

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

#### Hand Protection

Protective gloves

| Glove material | Breakthrough time | Glove thickness | EU standard | Glove comments        |
|----------------|-------------------|-----------------|-------------|-----------------------|
| Nitrile rubber | See manufacturers | -               | EN 374      | (minimum requirement) |
| Neoprene       | recommendations   |                 |             |                       |
| Natural rubber |                   |                 |             |                       |
| PVC            |                   |                 |             |                       |

#### Skin and body protection

Long sleeved clothing.

Inspect gloves before use. observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information) gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion. gloves with care avoiding skin contamination.

#### Respiratory Protection

No protective equipment is needed under normal use conditions.

### Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

**Recommended Filter type:** Particle filter

### Small scale/Laboratory use

Maintain adequate ventilation

**Recommended half mask:-** Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

### Environmental exposure controls

No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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

#### Physical State

Liquid

#### Appearance

#### Odor

No information available

#### Odor Threshold

No data available

#### Melting Point/Range

No data available

#### Softening Point

No data available

#### Boiling Point/Range

108 - 109 °C / 226.4 - 228.2 °F @ 0.1mmHg

#### Flammability (liquid)

No data available

#### Flammability (solid,gas)

Not applicable

Liquid

#### Explosion Limits

No data available

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|   |                          |                                   |
|---|--------------------------|-----------------------------------|
| Flash Point                             | 132 °C / 269.6 °F        | Method - No information available |
| Autoignition Temperature                | No data available        |                                   |
| Decomposition Temperature               | No data available        |                                   |
| pH                                      | No information available |                                   |
| Viscosity                               | No data available        |                                   |
| Water Solubility                        | Immiscible               |                                   |
| Solubility in other solvents            | No information available |                                   |
| Partition Coefficient (n-octanol/water) |                          |                                   |
| Vapor Pressure                          | No data available        |                                   |
| Density / Specific Gravity              | 1.103 g/cm3              | @ 20 °C                           |
| Bulk Density                            | Not applicable           | Liquid                            |
| Vapor Density                           | No data available        | (Air = 1.0)                       |
| Particle characteristics                | Not applicable (liquid)  |                                   |

## 9.2. Other information

|                   |            |
|-------------------|------------|
| Molecular Formula | C12 H12 O2 |
| Molecular Weight  | 188.23     |

## SECTION 10: STABILITY AND REACTIVITY

### 10.1. Reactivity

None known, based on information available

### 10.2. Chemical stability

Stable under normal conditions.

### 10.3. Possibility of hazardous reactions

|                          |                               |
|--------------------------|-------------------------------|
| Hazardous Polymerization | No information available.     |
| Hazardous Reactions      | None under normal processing. |

### 10.4. Conditions to avoid

Incompatible products. Excess heat.

### 10.5. Incompatible materials

Oxidizing agent.

### 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Product Information

#### (a) acute toxicity;

|            |  |
|------------|--|
| Oral       | Category 4   |
| Dermal     | Based on available data, the classification criteria are not met |
| Inhalation | Based on available data, the classification criteria are not met |

| Component                             | LD50 Oral                 | LD50 Dermal | LC50 Inhalation |
|---------------------------------------|---------------------------|-------------|-----------------|
| 1(3H)-Isobenzofuranone, 3-butylidene- | LD50 = 1850 mg/kg ( Rat ) | -           | -               |

|                                |                   |
|--------------------------------|-------------------|
| (b) skin corrosion/irritation; | No data available |
|--------------------------------|-------------------|

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|  |   |
|--|---|
| (c) serious eye damage/irritation;         | No data available   |
| (d) respiratory or skin sensitization;     |   |
| Respiratory                                | No data available   |
| Skin                                       | No data available   |
| (e) germ cell mutagenicity;                | No data available   |
| (f) carcinogenicity;                       | No data available   |
|  | There are no known carcinogenic chemicals in this product |
| (g) reproductive toxicity;                 | No data available   |
| (h) STOT-single exposure;                  | No data available   |
| (i) STOT-repeated exposure;                | No data available   |
| Target Organs                              | No information available.                                 |
| (j) aspiration hazard;                     | No data available   |
| Symptoms / effects, both acute and delayed | No information available.                                 |

## 11.2. Information on other hazards

|  |   |
|--|---|
| <b>Endocrine Disrupting Properties</b> | Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors. |
|--|---|

## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

|                            |   |
|----------------------------|---|
| <b>Ecotoxicity effects</b> | Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants. |
|----------------------------|---|

### 12.2. Persistence and degradability

|                    |   |
|--------------------|---|
| <b>Persistence</b> | Immiscible with water, Persistence is unlikely, based on information available. |
|--------------------|---|

|   |  |
|---|--|
| <u><b>12.3. Bioaccumulative potential</b></u> | May have some potential to bioaccumulate |
|---|--|

### 12.4. Mobility in soil

Spillage unlikely to penetrate soil The product is insoluble and sinks in water The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces Is not likely mobile in the environment due its low water solubility. Will likely be mobile in the environment due to its volatility.

### 12.5. Results of PBT and vPvB assessment

No data available for assessment.

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## 12.6. Endocrine disrupting properties

### Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

## 12.7. Other adverse effects

### Persistent Organic Pollutant Ozone Depletion Potential

This product does not contain any known or suspected substance  
This product does not contain any known or suspected substance

## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

#### Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

#### Contaminated Packaging

Dispose of this container to hazardous or special waste collection point.

#### European Waste Catalogue (EWC)

According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

#### Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

#### Switzerland - Waste Ordinance

Disposal should be in accordance with applicable regional, national and local laws and regulations. Ordinance on the Avoidance and the Disposal of Waste (Waste Ordinance, ADWO) SR 814.600  
<https://www.fedlex.admin.ch/eli/cc/2015/891/en>

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

Not regulated

#### 14.1. UN number

#### 14.2. UN proper shipping name

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

#### 14.4. Packing group

### ADR

Not regulated

#### 14.1. UN number

#### 14.2. UN proper shipping name

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

#### 14.4. Packing group

### IATA

Not regulated

#### 14.1. UN number

#### 14.2. UN proper shipping name

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

#### 14.4. Packing group

#### 14.5. Environmental hazards

No hazards identified

#### 14.6. Special precautions for user

No special precautions required.

#### 14.7. Maritime transport in bulk according to IMO instruments

Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION



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

### International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

| Component                             | CAS No   | EINECS    | ELINCS | NLP | IECSC | TCSI | KECL | ENCS | ISHL |
|---------------------------------------|----------|-----------|--------|-----|-------|------|------|------|------|
| 1(3H)-Isobenzofuranone, 3-butyldiene- | 551-08-6 | 208-991-3 | -      | -   | X     | X    | -    | -    | X    |

| Component                             | CAS No   | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|---------------------------------------|----------|------|---|-----|------|------|-------|-------|
| 1(3H)-Isobenzofuranone, 3-butyldiene- | 551-08-6 | X    | ACTIVE  | X   | -    | X    | X     | X     |

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

### Authorisation/Restrictions according to EU REACH

Not applicable

| Component                             | CAS No   | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|---------------------------------------|----------|---|---|---|
| 1(3H)-Isobenzofuranone, 3-butyldiene- | 551-08-6 | -   | -   | -   |

### Seveso III Directive (2012/18/EC)

| Component                             | CAS No   | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements |
|---------------------------------------|----------|---|--|
| 1(3H)-Isobenzofuranone, 3-butyldiene- | 551-08-6 | Not applicable  | Not applicable   |

### Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

### Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

### National Regulations

**UK** - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

### WGK Classification

Water endangering class = 3 (self classification)

### Swiss Regulations

Article 4 para. 4 of the Ordinance on the protection of young people in the workplace (SR 822.115) and Article 1 lit. f of the EAER regulation on hazardous work and young people (SR 822.115.2).

Take note on Article 13 Maternity Ordinance (SR 822.111.52) with regards expectant and nursing mothers.

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## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

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

H302 - Harmful if swallowed

### Legend

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

### Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (volatile organic compound)

### Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

### Prepared By

Health, Safety and Environmental Department

### Revision Date

23-Feb-2024

### Revision Summary

New emergency telephone response service provider.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006. COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No 1907/2006 .**

**For Switzerland - Compiled in accordance with the technical provisions referred to in Annex 2, Number 3, ChemO (SR 813.11 - Ordinance on Protection against Dangerous Substances and Preparations).**

### Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

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**End of Safety Data Sheet**