

## 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  
Avocado Research Chemicals Ltd.  
(Part of Thermo Fisher Scientific)  
Shore Road, Heysham  
Lancashire, LA3 2XY,  
United Kingdom  
Office Tel: +44 (0) 1524 850506  
Office Fax: +44 (0) 1524 850608

E-mail address 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

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

#### Physical hazards

Based on available data, the classification criteria are not met

#### Health hazards

Acute oral toxicity

Category 4 (H302)

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## 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 - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
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.

#### Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

#### Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

#### Ingestion

Clean mouth with water and drink afterwards plenty of water.

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**Inhalation** Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

**Self-Protection of the First Aider** 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**

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

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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      Class 10  
Storage Class (LGK) (Germany)

### 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

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

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 recommendations		EN 374	(minimum requirement)
Neoprene				
Natural rubber				

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PVC	-
<b>Skin and body protection</b>	Long sleeved clothing.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.  
(Refer to manufacturer/supplier for information)

Ensure 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.

Remove 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

#### 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)

No data available

#### 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

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## 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**  
**Hazardous Reactions**

No information available.  
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

#### (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

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(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

Endocrine Disrupting Properties	Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.
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## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

Ecotoxicity effects	Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.
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### 12.2. Persistence and degradability

Persistence	Immiscible with water, Persistence is unlikely, based on information available.
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### 12.3. Bioaccumulative potential

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.

### 12.6. Endocrine disrupting properties

Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
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### 12.7. Other adverse effects

Persistent Organic Pollutant	This product does not contain any known or suspected substance
Ozone Depletion Potential	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.

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## 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.

## 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

### 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-butylidene-	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-butylidene-	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) -	REACH (1907/2006) -	REACH Regulation (EC
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		Annex XIV - Substances Subject to Authorization	Annex XVII - Restrictions on Certain Dangerous Substances	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)

## 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/NDL** - 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

**TWA** - Time Weighted Average

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

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**RPE** - Respiratory Protective Equipment  
**LC50** - Lethal Concentration 50%  
**NOEC** - No Observed Effect Concentration  
**PBT** - Persistent, Bioaccumulative, Toxic

**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

**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)

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>  
Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**Training Advice**

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

<b>Prepared By</b>	Health, Safety and Environmental Department
<b>Revision Date</b>	23-Feb-2024
<b>Revision Summary</b>	New emergency telephone response service provider.

**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.**

**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

**End of Safety Data Sheet**