Thermo Fisher SCIENTIFIC

SAFETY DATA SHEET

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Revision Date 22-Apr-2024
Version 3

ALFAAA10114

Isobutyl benzoate

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明: 苯甲酸异丁酯 Product Description: Isobutyl benzoate

Cat No.: A10114

Synonyms 2-Methylpropyl Benzoate.

CAS No 120-50-3 Molecular Formula C11 H14 O2

Supplier Avocado Research Chemicals Ltd.

(Part of Thermo Fisher Scientific)

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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

E-mail address begel.sdsdesk@thermofisher.com

Recommended Use Laboratory chemicals. Uses advised against No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State Appearance Odor

Liquid Colorless No information available

Emergency Overview

The product contains no substances which at their given concentration are considered to be hazardous to health.

Classification of the substance or mixture

Based on available data, the classification criteria are not met

Label Elements

None required

Physical and Chemical Hazards

None identified.

Health Hazards

The product contains no substances which at their given concentration are considered to be hazardous to health.

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil. The product evaporates slowly.

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This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %		
Benzoic acid, 2-methylpropyl ester	120-50-3	98		

SECTION 4. FIRST AID MEASURES

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 soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.

Inhalation

Remove from exposure, lie down. Remove to fresh air.

Ingestion

Clean mouth with water. Get medical attention.

Most important symptoms and effects

No information available.

Self-Protection of the First Aider

No special precautions required.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES

Suitable Extinguishing Media

Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

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

Protective Equipment and Precautions 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

Personal Precautions

Ensure adequate ventilation.

Environmental Precautions

See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

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Sweep up and shovel into suitable containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE

Handling

Avoid contact with skin and eyes. Do not breathe mist/vapors/spray.

Storage

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

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters

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

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

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.

Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure
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

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Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Liquid

(Air = 1.0)

Liquid

Appearance Colorless **Physical State** Liquid

No information available Odor **Odor Threshold** No data available No information available pН No data available **Melting Point/Range**

Softening Point No data available 240 - 242 °C / 464 - 467.6 °F **Boiling Point/Range**

96 °C / 204.8 °F **Flash Point** Method - No information available

Evaporation Rate No data available Flammability (solid,gas) Not applicable

Explosion Limits No data available

Vapor Pressure No data available

Vapor Density No data available

Specific Gravity / Density 0.999 **Bulk Density** Not applicable

Water Solubility Insoluble

No information available Solubility in other solvents

Partition Coefficient (n-octanol/water)

No data available **Autoignition Temperature** No data available **Decomposition Temperature Viscosity** No data available **Explosive Properties** No information available **Oxidizing Properties** No information available

C11 H14 O2 Molecular Formula **Molecular Weight** 178.23

SECTION 10. STABILITY AND REACTIVITY

Stability Stable.

Hazardous Reactions No information available.

Hazardous Polymerization Hazardous polymerization does not occur.

Conditions to Avoid Heat, flames and sparks. Materials to avoid Strong oxidizing agents.

Hazardous Decomposition Products Carbon monoxide (CO). Carbon dioxide (CO2).

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

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Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzoic acid, 2-methylpropyl ester	LD50 = 5600 mg/kg (Rat)		

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;

RespiratoryNo data availableSkinNo 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

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects,both acute and No information available

delayed

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects

Persistence and Degradability

Persistence Insoluble in water, May persist, based on information available.

Bioaccumulative Potential May have some potential to bioaccumulate

Mobility in soil Spillage unlikely to penetrate soil The product evaporates slowly Is not likely mobile in the

environment due its low water solubility Spillage unlikely to penetrate soil

Endocrine Disruptor Information

Persistent Organic Pollutant
Ozone Depletion Potential

This product does not contain any known or suspected endocrine disruptors

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

SECTION 13. DISPOSAL CONSIDERATIONS

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Waste from Residues/Unused

Products

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Consult local, regional, and national hazardous waste regulations to

ensure complete and accurate classification.

Contaminated Packaging Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use

empty containers.

Other Information Waste codes should be assigned by the user based on the application for which the product

was used.

SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport Not Regulated

IMDG/IMO Not regulated

IATA Not regulated

Special Precautions for User No special precautions required

SECTION 15. REGULATORY INFORMATION

International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)		TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Benzoic acid,	-	-	X	Х	204-401-3	Х	X	Х	X	Х	X	KE-21440
2-methylpropyl ester												

National Regulations

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department

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Revision Summary New emergency telephone response service provider.

Training Advice

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

Legend

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CAS - Chemical Abstracts Service

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

IMO/IMDG - International Maritime Organization/International Maritime

MARPOL - International Convention for the Prevention of Pollution from

EINECS/ELINCS - European Inventory of Existing Commercial Chemical **DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances/EU List of Notified Chemical Substances

Substances List

PICCS - Philippines Inventory of Chemicals and Chemical Substances

ENCS - Japa

IECSC - Chinese Inventory of Existing Chemical Substances **KECL** - Korean Existing and Evaluated Chemical Substances

ENCS - Japanese Existing and New Chemical Substances
AICS - Australian Inventory of Chemical Substances
NZIOC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit TWA - Time Weighted Average

ACGIH - American Conference of Governmental Industrial Hygienists IARC - International Agency for Research on Cancer

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

LC50 - Lethal Concentration 50%EC50 - Effective Concentration 50%NOEC - No Observed Effect ConcentrationPOW - Partition coefficient Octanol:WaterPBT - Persistent, Bioaccumulative, ToxicvPvB - very Persistent, very Bioaccumulative

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

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

Dangerous Goods by Road

OECD - Organisation for Economic Co-operation and Development

ATE - Acute Toxicity Estimate

BCF - Bioconcentration factor 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

Disclaimer

Dangerous Goods Code

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