

according to Regulation UK SI 2019/758 and UK SI 2020/1577 as amended

Revision Date 25-Sep-2023 **Revision Number** 6

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

1.1. Product identifier

Product Description: Isophthalic acid

Cat No.: 122650000; 122650020; 122650050 **Synonyms** 1,3-Benzenedicarboxylic acid

CAS No 121-91-5 C8 H6 O4 Molecular Formula

REACH registration number 01-2119488938-12

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

Recommended Use Laboratory chemicals.

Sector of use SU3 - Industrial uses: Uses of substances as such or in preparations at industrial sites

Product category PC21 - Laboratory chemicals

Process categories PROC15 - Use as a laboratory reagent

Environmental release category ERC6a - Industrial use resulting in manufacture of another substance (use of intermediates)

Uses advised against No Information available

1.3. Details of the supplier of the safety data sheet

Company

UK entity/business name Fisher Scientific UK

Bishop Meadow Road,

Loughborough, Leicestershire LE11 5RG, United Kingdom

EU entity/business name

Thermo Fisher Scientific

Janssen Pharmaceuticalaan 3a, 2440 Geel, Belgium

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

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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

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Health hazards

Based on available data, the classification criteria are not met

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements

None required

2.3. Other hazards

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB)

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
Į:	sophthalic acid	121-91-5	EEC No. 204-506-4	99	-

REACH registration number	01-2119488938-12
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Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of 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.

Ingestion Clean mouth with water. Get medical attention.

Inhalation Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial

respiration. Get medical attention.

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Self-Protection of the First Aider No special precautions required.

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

No information available.

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

Water spray. Carbon dioxide (CO₂). Dry chemical. Alcohol resistant foam.

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

Thermal decomposition can lead to release of irritating gases and vapors, Carbon monoxide (CO), Carbon dioxide (CO₂).

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.

6.2. Environmental precautions

See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

Sweep up and shovel into suitable 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

Avoid contact with skin and eyes. Do not breathe dust.

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

Technical Rules for Hazardous Substances (TRGS) 510 Class 11 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

List source(s):

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)

See table for values

Component	Component Acute effects local (Dermal) s		Chronic effects local (Dermal)	Chronic effects systemic (Dermal)	
Isophthalic acid 121-91-5 (99)				DNEL = 25mg/kg bw/day	

Component		Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
Isophthalic ac 121-91-5 (99	-				DNEL = 8.8mg/m ³

Predicted No Effect Concentration (PNEC)

See values below.

Component	Fresh water	Fresh water sediment	Water Intermittent	Microorganisms in sewage treatment	, ,
Isophthalic acid 121-91-5 (99)	PNEC = 0.907mg/L	PNEC = 1.246mg/kg sediment dw	PNEC = 9.07mg/L	PNEC = 16mg/L	PNEC = 1.69mg/kg soil dw

Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
Isophthalic acid	PNEC =	PNEC =			

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121-91-5 (99)	0.0907mg/L	0.1246mg/kg		
		sediment dw		

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

Skin and body protection 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 Powder Solid

Appearance Off-white Odor Odorless

Odor Threshold No data available

Melting Point/Range 341 - 343 °C / 645.8 - 649.4 °F

Softening Point No data available
Boiling Point/Range No information available

Flammability (liquid) Not applicable Solid

Flammability (solid,gas)

Explosion Limits

No information available

No data available

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Flash Point No information available Method - No information available

Autoignition Temperature

Decomposition Temperature

pH

650 °C / 1202 °F

No data available

No information available

Viscosity Not applicable Solid

Water Solubility 0.01g/100ml (25 C) practically insoluble

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Componentlog PowIsophthalic acid2.32

Vapor Pressure
Density / Specific Gravity
Bulk Density
Vapor Density
No data available
No data available
No data available
Not applicable

Particle characteristics No data available

9.2. Other information

Molecular Formula C8 H6 O4 Molecular Weight 166.13

Evaporation Rate Not applicable - Solid

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 PolymerizationNo information available.Hazardous ReactionsNo information available.

10.4. Conditions to avoid

Incompatible products.

10.5. Incompatible materials

Strong oxidizing agents. Strong bases.

10.6. Hazardous decomposition products

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

Solid

monoxide (CO). Carbon dioxide (CO2).

SECTION 11: TOXICOLOGICAL INFORMATION

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

Product Information No acute toxicity information is available for this product

(a) acute toxicity;

OralBased on available data, the classification criteria are not metDermalBased on available data, the classification criteria are not metInhalationBased on available data, the classification criteria are not met

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Component	LD50 Oral	LD50 Dermal	LC50 Inhalation		
Isophthalic acid	10400 mg/kg (Rat)	> 2000 mg/kg (Rabbit)	LC50 > 11370 mg/m³ (Rat) 4 h		

(b) skin corrosion/irritation; Based on available data, the classification criteria are not met

(c) serious eye damage/irritation; Based on available data, the classification criteria are not met

(d) respiratory or skin sensitization;

Respiratory Skin Based on available data, the classification criteria are not met Based on available data, the classification criteria are not met

(e) germ cell mutagenicity; Based on available data, the classification criteria are not met

(f) carcinogenicity; Based on available data, the classification criteria are not met

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; Based on available data, the classification criteria are not met

(h) STOT-single exposure; Based on available data, the classification criteria are not met

(i) STOT-repeated exposure; Based on available data, the classification criteria are not met

Target Organs None known.

(j) aspiration hazard; Not applicable

Solid

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

Symptoms / effects,both acute and No information available.

delayed

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.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effectsContains no substances known to be hazardous to the environment or that are not

degradable in waste water treatment plants.

12.2. Persistence and degradability

Persistence Persistence is unlikely.

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12.3. Bioaccumulative potential Bioaccumulation is unlikely
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Component	log Pow	Bioconcentration factor (BCF)
Isophthalic acid	2.32	No data available

12.4. Mobility in soil Spillage unlikely to penetrate soil . Is not likely mobile in the environment due its low water

solubility.

12.5. Results of PBT and vPvB

assessment

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent

and very bioaccumulative (vPvB).

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

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.

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.

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

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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

Component

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)

0 0 111 0 1110111					•				
Isophthalic acid	121-91-5	204-506-4	-	-	X	X	KE-02189	Х	X
Component	CAS No	TSCA	TSCA In	ventory	DSL	NDSL	AICS	NZIoC	PICCS
-			notific	ation -					

EINECS ELINCS NLP IECSC TCSI KECL ENCS

Isophthalic acid 121-91-5 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

CAS No

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization		REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Isophthalic acid	121-91-5	-	-	-

Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) -	Seveso III Directive (2012/18/EC) -	
		Qualifying Quantities for Major Accident		
		Notification	Requirements	
Isophthalic acid	121-91-5	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

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work .

National Regulations

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

WGK Classification

Water endangering class = 2 (self classification)

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Isophthalic acid	WGK1	

Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
Isophthalic acid	Prohibited and Restricted		
121-91-5 (99)	Substances		Į.

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

Legend

CAS - Chemical Abstracts Service

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

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

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

KECL - Korean Existing and Evaluated 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%

VOC - (Volatile Organic Compound)

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

Key literature references and sources for data

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

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

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Training Advice

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

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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