

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

Creation Date 16-Nov-2010 Revision Date 22-Sep-2023 Revision Number 5

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

#### 1.1. Product identifier

Product Description: 4-Methyl-3-nitrobenzoic acid

Cat No.: 165990000; 165990250; 165991000; 165995000

Synonyms 3-Nitro-p-toluic acid

 CAS No
 96-98-0

 EC No
 202-549-3

 Molecular Formula
 C8 H7 N O4

#### 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

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

## **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**

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Skin Corrosion/Irritation Category 2 (H315)
Serious Eye Damage/Eye Irritation Category 2 (H319)

Specific target organ toxicity - (single exposure)

Category 3 (H335)

#### **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**

H319 - Causes serious eye irritation

H315 - Causes skin irritation

H335 - May cause respiratory irritation

## **Precautionary Statements**

P280 - Wear protective gloves/protective clothing/eye protection/face protection

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

#### 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
Benzoic acid, 4-methyl-3-nitro-	96-98-0	EEC No. 202-549-3	>95	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319)

Full text of Hazard Statements: see section 16

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## **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** Get medical attention. Wash off immediately with plenty of water for at least 15 minutes.

**Ingestion** Clean mouth with water and drink afterwards plenty of water. Get medical attention if

symptoms occur.

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

**Self-Protection of the First Aider** Use personal protective equipment as 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**

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**

Nitrogen oxides (NOx), 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

Use personal protective equipment as required. Ensure adequate ventilation. Avoid dust formation.

## 6.2. Environmental precautions

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

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

Sweep up and shovel into suitable containers for disposal. 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. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

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

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

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**

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.

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#### 8.2. Exposure controls

#### **Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

**Eve Protection** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

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

Long sleeved clothing. Skin and body protection

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** When workers are facing concentrations above the exposure limit they must use

appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used

and maintained properly

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits Large scale/emergency use

> are exceeded or if irritation or other symptoms are experienced Recommended Filter type: Particulates filter conforming to EN 143

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure Small scale/Laboratory use

limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Particle filtering: EN149:2001 When RPE is used a face piece Fit Test should be conducted

**Environmental exposure controls** No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

## 9.1. Information on basic physical and chemical properties

Powder Solid **Physical State** 

**Appearance** Off-white

No information available Odor **Odor Threshold** No data available

187 - 190 °C / 368.6 - 374 °F Melting Point/Range

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

Not applicable Flammability (liquid) Solid

Flammability (solid,gas) No information available

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Solid

Solid

**Explosion Limits** No data available

No information available Method - No information available **Flash Point** 

**Autoignition Temperature** No data available **Decomposition Temperature** No data available No information available pН

Viscosity Not applicable

Slightly soluble **Water Solubility** 

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Component log Pow Benzoic acid, 4-methyl-3-nitro-1.65

**Vapor Pressure** No information available Density / Specific Gravity No data available

**Bulk Density** No data available Not applicable **Vapor Density** 

Particle characteristics No data available

9.2. Other information

C8 H7 N O4 Molecular Formula **Molecular Weight** 181.15

**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 recommended storage conditions.

10.3. Possibility of hazardous reactions

No information available. **Hazardous Polymerization Hazardous Reactions** None under normal processing.

10.4. Conditions to avoid

Incompatible products. Excess heat. Avoid dust formation.

10.5. Incompatible materials

Strong oxidizing agents. Strong bases.

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon 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;

Oral No data available **Dermal** No data available Inhalation No data available

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Category 2 (b) skin corrosion/irritation;

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory Skin

No data available

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; Category 3

Results / Target organs Respiratory system.

(i) STOT-repeated exposure; No data available

**Target Organs** No information available.

(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 effects** 

Component	Freshwater Fish	Water Flea	Freshwater Algae
Benzoic acid, 4-methyl-3-nitro-	LC50: > 100 mg/L, 96h static (Danio rerio)		

12.2. Persistence and degradability

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

#### 4-Methyl-3-nitrobenzoic acid

**12.3. Bioaccumulative potential** May have some potential to bioaccumulate

Componentlog PowBioconcentration factor (BCF)Benzoic acid, 4-methyl-3-nitro-1.65No 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

No data available for assessment.

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

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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.

## **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

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#### 4-Methyl-3-nitrobenzoic acid

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)

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Benzoic acid, 4-methyl-3-nitro-	96-98-0	202-549-3	-	-	Х	X	-	Х	Х
Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Benzoic acid, 4-methyl-3-nitro-	96-98-0	X	ACTIVE	1	X	ı	-	-

Legend: X - Listed '-' - Not Listed KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

96-98-0

## Authorisation/Restrictions according to EU REACH

Component	CAS No	REACH (1907/2006) -	REACH (1907/2006) -	REACH Regulation (EC
		Annex XIV - Substances	Annex XVII - Restrictions	1907/2006) article 59 -
		Subject to Authorization	on Certain Dangerous	Candidate List of
			Substances	Substances of Very High
				Concern (SVHC)

Not applicable

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

Benzoic acid, 4-methyl-3-nitro-

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
Benzoic acid, 4-methyl-3-nitro-	96-98-0	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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#### 4-Methyl-3-nitrobenzoic acid

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#### **National Regulations**

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

**WGK Classification** See table for values

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Benzoic acid, 4-methyl-3-nitro-	WGK1	

#### 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

H315 - Causes skin irritation

H319 - Causes serious eye irritation H335 - May cause respiratory irritation

#### Legend

**CAS** - Chemical Abstracts Service

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

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

EINECS/ELINCS - European Inventory of Existing Commercial Chemical 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

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.

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Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

**Creation Date** 16-Nov-2010 **Revision Date** 22-Sep-2023 **Revision Summary** Not applicable.

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**