

Revision Date 05-Sep-2023 Revision Number 5

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

#### 1.1. Product identifier

Product Description: 3-(1H-Pyrrol-1-yl)benzoic acid

Cat No.: CC21901CB; CC21901DA; CC21901ZZ; CC21901FL; CC21901R3; CC21901SC

Molecular Formula C11 H9 N 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

**EU entity/business name** Thermo Fisher Scientific Janssen Pharmaceuticalaan 3a

2440 Geel, Belgium

UK entity/business name

Thermo Fisher Scientific (Heysham),

Shore Road,

Port of Heysham Industrial Park, Heysham, Lancashire, LA3 2XY

United Kingdom

Swiss distributor - Fisher Scientific AG Neuhofstrasse 11. CH 4153 Reinach

Tel: +41 (0) 56 618 41 11

e-mail - infoch@thermofisher.com

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

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

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#### CLP Classification - Regulation (EC) No 1272/2008

#### **Physical hazards**

Based on available data, the classification criteria are not met

#### **Health hazards**

Skin Corrosion/Irritation Serious Eye Damage/Eye Irritation Specific target organ toxicity - (single exposure) Category 2 (H315) Category 2 (H319) 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**

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

#### **Precautionary Statements**

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

P337 + P313 - If eye irritation persists: Get medical advice/attention

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

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

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

P332 + P313 - If skin irritation occurs: Get medical advice/attention

## 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
3-(1H-Pyrrol-1-yl)benzoic acid	61471-45-2		97	STOT SE 3 (H335)

## 3-(1H-Pyrrol-1-yl)benzoic acid

		Skin Irrit. 2 (H315) Eye Irrit. 2 (H319)

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.

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get **Eve Contact** 

medical attention.

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, **Skin Contact** 

call a physician.

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

symptoms occur.

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

symptoms occur.

Ensure that medical personnel are aware of the material(s) involved, take precautions to Self-Protection of the First Aider

protect themselves and prevent spread of contamination.

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 (CO<sub>2</sub>). Dry chemical. Chemical 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

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protective gear.

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

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

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

#### 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

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. 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

Storage Class (LGK) (Germany)

Storage Class/LGK 11

Switzerland - Storage of hazardous substances

Storage class -

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 SC 11/13

#### 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

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#### **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.

MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

#### 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**

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

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

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber	See manufacturers	-	EN 374	(minimum requirement)
Butyl rubber	recommendations			
Nitrile rubber				
Neoprene				
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** When workers are facing concentrations above the exposure limit they must use

appropriate certified respirators.

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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:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN

Solid

Solid

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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

**Physical State** Solid

**Appearance** No information available Odor No information available

**Odor Threshold** No data available

180 - 181 °C / 356 - 357.8 °F Melting Point/Range

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

Not applicable Flammability (liquid)

Flammability (solid,gas) No information available No data available **Explosion Limits** 

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

**Autoignition Temperature** No data available **Decomposition Temperature** No data available рΗ No data available Viscosity Not applicable

Soluble in water Water Solubility

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

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

Solid

**Particle characteristics** No data available

#### 9.2. Other information

C11 H9 N O2 Molecular Formula **Molecular Weight** 187.2

**Evaporation Rate** Not applicable - Solid

## **SECTION 10: STABILITY AND REACTIVITY**

10.1. Reactivity None known, based on information available

#### 10.2. Chemical stability

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Stable under normal 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.

10.5. Incompatible materials

Bases. Strong oxidizing agents. Amines. Reducing Agent.

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). 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** No acute toxicity information is available for this product

(a) acute toxicity;

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

Category 2 (b) skin corrosion/irritation;

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory No data available No data available Skin

No data available (e) germ cell mutagenicity;

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

Category 3 (h) STOT-single exposure:

Respiratory system. Results / Target organs

(i) STOT-repeated exposure; No data available

No information available. **Target Organs** 

(j) aspiration hazard; Not applicable

Solid

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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

Contains no substances known to be hazardous to the environment or that are not **Ecotoxicity effects** 

degradable in waste water treatment plants.

12.2. Persistence and degradability

**Persistence** Soluble in water. Persistence is unlikely, based on information available.

12.3. Bioaccumulative potential Bioaccumulation is unlikely

The product is water soluble, and may spread in water systems Will likely be mobile in the 12.4. Mobility in soil

environment due to its water solubility. Highly mobile in soils

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 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

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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

No hazards identified 14.5. Environmental hazards

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
3-(1H-Pyrrol-1-yl)benzoic acid	61471-45-2	-	-	-	-	-	-	-	1

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
3-(1H-Pyrrol-1-yl)benzoic acid	61471-45-2	-	-	-	-	-	-	-

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

#### 3-(1H-Pyrrol-1-yl)benzoic acid

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	J	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
3-(1H-Pyrrol-1-yl)benzoic acid	61471-45-2	-	-	-

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
3-(1H-Pyrrol-1-yl)benzoic acid	61471-45-2	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.

#### 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

**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 - Japanese Existing and New Chemical Substances

ALCS - Australian Inventory of Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

NZIOC - New Zealand Inventory of Chemicals

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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

ICAO/IATA - International Civil Aviation Organization/International Air

MARPOL - International Convention for the Prevention of Pollution from

Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

**Transport Association** 

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

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.

Ships

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.

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SDS sections updated, 1, 2, 9, 11, 12, 15, 16. **Revision Summary** 

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

**End of Safety Data Sheet**