

according to Regulation (EC) No. 1907/2006

Revision Date 05-Sep-2023

**Revision Number** 3

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

#### 1.1. Product identifier

Product Description: Pentafluorophenyl 3-(1-methyl-1H-pyrazol-3-yl)benzoate

Cat No. : CC60626CB; CC60626DA; CC60626ZZ

Molecular Formula C17 H9 F5 N2 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

Revision Date 05-Sep-2023

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

#### **Physical hazards**

Based on available data, the classification criteria are not met

#### **Health hazards**

Acute oral toxicity

Acute dermal toxicity

Acute Inhalation Toxicity - Dusts and Mists

Serious Eye Damage/Eye Irritation

Specific target organ toxicity - (single exposure)

Category 4 (H312)

Category 4 (H332)

Category 4 (H332)

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

H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

#### **Precautionary Statements**

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting

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

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

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

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

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
Pentafluorophenyl 3-(1-methyl-1H-pyrazol-3-yl)benzoate	910037-11-5		> 97	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332)

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. Get medical attention if

symptoms occur.

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

symptoms occur.

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

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 (CO2). 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

#### Pentafluorophenyl 3-(1-methyl-1H-pyrazol-3-yl)benzoate

Revision Date 05-Sep-2023

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

#### **Hazardous Combustion Products**

Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO2), Gaseous hydrogen fluoride (HF), Fluorine.

#### 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. 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 - SC 11/13

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

Page 4/12

#### 7.3. Specific end use(s)

Use in laboratories

#### **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

#### Pentafluorophenyl 3-(1-methyl-1H-pyrazol-3-yl)benzoate

#### 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

#### **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
Nitrile rubber Neoprene	See manufacturers recommendations	-	EN 374	(minimum requirement)
Natural rubber	recommendations			
PVC				

**Skin and body protection** Long sleeved clothing.

MAYCC60626

## Pentafluorophenyl 3-(1-methyl-1H-pyrazol-3-yl)benzoate

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.

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

appropriate certified respirators.

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

Revision Date 05-Sep-2023

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.

Solid

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

Solid **Physical State** 

**Appearance** Off-white

Odor No information available

**Odor Threshold** No data available

**Melting Point/Range** 126 - 127 °C / 258.8 - 260.6 °F

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

Flammability (liquid) Not applicable

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 Ha No data available Not applicable **Viscosity** 

Solid

Water Solubility Soluble in water

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

**Vapor Pressure** No data available **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

C17 H9 F5 N2 O2 Molecular Formula

**Molecular Weight** 368.26

**Evaporation Rate** Not applicable - Solid

Pentafluorophenyl 3-(1-methyl-1H-pyrazol-3-yl)benzoate

Revision Date 05-Sep-2023

## **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 ReactionsNone under normal processing.

10.4. Conditions to avoid

Incompatible products.

10.5. Incompatible materials

Strong oxidizing agents. Strong reducing agents.

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO2). Gaseous hydrogen

fluoride (HF). Fluorine.

## **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 Category 4
Inhalation Category 4

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(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; Category 3

Pentafluorophenyl 3-(1-methyl-1H-pyrazol-3-yl)benzoate

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** Do not empty into drains.

12.2. Persistence and degradability

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

**12.3. Bioaccumulative potential** Bioaccumulation is unlikely

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

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 Waste is classified as hazardous. Dispose of in accordance with the European Directives

Pentafluorophenyl 3-(1-methyl-1H-pyrazol-3-yl)benzoate

Revision Date 05-Sep-2023

**Products** 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.

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

**14.1. UN number** UN2811

**14.2. UN proper shipping name** Toxic solid, organic, n.o.s.

14.3. Transport hazard class(es) 6.1 14.4. Packing group III

#### ADR

**14.1. UN number** UN2811

**14.2. UN proper shipping name** Toxic solid, organic, n.o.s.

14.3. Transport hazard class(es) 6.1 14.4. Packing group III

#### <u>IATA</u>

**14.1. UN number** UN2811

**14.2. UN proper shipping name** Toxic solid, organic, n.o.s.

**14.3. Transport hazard class(es)** 6.1 **14.4. Packing group** III

**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
Pentafluorophenyl	910037-11-5	-	-	-	-	-	-	-	-
3-(1-methyl-1H-pyrazol-3-yl)benzo									
ate									

#### Pentafluorophenyl 3-(1-methyl-1H-pyrazol-3-yl)benzoate

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Pentafluorophenyl	910037-11-5	-	-	-	-	-	-	-
3-(1-methyl-1H-pyrazol-3-yl)benzo								
ate								

**Legend:** X - Listed '-' - Not Listed **KECL** - NIER number or KE n

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) - Annex XIV - Substances Subject to Authorization		REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Pentafluorophenyl 3-(1-methyl-1H-pyrazol-3-yl)benzoat e	910037-11-5	-	-	-

#### 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
Pentafluorophenyl 3-(1-methyl-1H-pyrazol-3-yl)	910037-11-5	Not applicable	Not applicable
benzoate			

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

Revision Date 05-Sep-2023

## **SECTION 16: OTHER INFORMATION**

#### Full text of H-Statements referred to under sections 2 and 3

H302 - Harmful if swallowed

H312 - Harmful in contact with skin

H332 - Harmful if inhaled

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

PICCS - Philippines Inventory of Chemicals and Chemical Substances

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

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.

**Revision Date** 05-Sep-2023

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,

Pentafluorophenyl 3-(1-methyl-1H-pyrazol-3-yl)benzoate

Revision Date 05-Sep-2023

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**