

Creation Date 20-Sep-2010 Revision Date 01-Sep-2023 **Revision Number** 6

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

1.1. Product identifier

Product Description: Hydrocinnamoyl chloride

Cat No.: SB01152DA; SB01152EA; SB01152EB; SB01152EE; SB01152ZZ

Synonyms 3-Phenylpropionyl chloride

CAS No 645-45-4 EC No 211-443-6 Molecular Formula C9 H9 CI O

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

Laboratory chemicals. **Recommended Use** 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

begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

E-mail address

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

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2.1. Classification of the substance or mixture

CLP Classification - Regulation (EC) No 1272/2008

Physical hazards

Based on available data, the classification criteria are not met

Health hazards

Acute Inhalation Toxicity - Vapors Category 3 (H331) Skin Corrosion/Irritation Category 2 (H315)

Environmental hazards

Chronic aquatic toxicity Category 3 (H412)

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Danger

Hazard Statements

H331 - Toxic if inhaled

H315 - Causes skin irritation

H412 - Harmful to aquatic life with long lasting effects

Precautionary Statements

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

P311 - Call a POISON CENTER or doctor/physician

P280 - Wear protective gloves/protective clothing

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

2.3. Other hazards

Decomposes in contact with water

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

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Component	CAS NO	EC NO	weight %	1272/2008
Benzenepropanoyl chloride	645-45-4	EEC No. 211-443-6	<=100	Skin Irrit. 2 (H315) Acute Tox. 3 (H331) Aquatic Chronic 3 (H412)

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

General Advice Show this safety data sheet to the doctor in attendance. Immediate medical attention is

required.

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. Immediate medical

attention is required.

Ingestion Do NOT induce vomiting. Call a physician or poison control center immediately.

Inhalation Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth

method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device.

Immediate medical attention is required.

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. Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and

danger of perforation

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

CO₂, dry chemical, dry sand, alcohol-resistant foam.

Extinguishing media which must not be used for safety reasons

Contact with water liberates toxic gas.

5.2. Special hazards arising from the substance or mixture

Contact with water liberates toxic gas.

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Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO2), Hydrogen chloride gas.

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

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation. Use personal protective equipment as required. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas.

6.2. Environmental precautions

Should not be released into the environment. Do not flush into surface water or sanitary sewer system.

6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Do not expose spill to water.

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. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Do not allow contact with water.

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 away from water or moist air. Keep containers tightly closed in a dry, cool and well-ventilated place. Corrosives area.

Technical Rules for Hazardous Substances (TRGS) 510 Storage Class (LGK) (Germany)

Storage Class/LGK 6.1C

Switzerland - Storage of hazardous substances

Storage class - SC 6.1

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

7.3. Specific end use(s)

Use in laboratories

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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

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.

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

Use only under a chemical fume hood. 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 Natural rubber PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

Skin and body protectionWear appropriate protective gloves and clothing to prevent skin exposure.

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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.

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

and maintained properly

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: Organic gases and vapours filter Type A Brown conforming to

EN14387

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

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

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

@ 11 mmHg

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When RPE is used a face piece Fit Test should be conducted

Environmental exposure controls Prevent product from entering drains.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State Liquid

AppearanceLight yellowOdorpungent

Odor Threshold No data available

Melting Point/Range -6 - -5.00 °C / 21.2 - 23 °F

Softening Point

Boiling Point/Range

107 °C / 224.6 °F

Flammability (liquid)

No data available

Flammability (solid,gas) Not applicable Liquid

Explosion Limits No data available

Flash Point 108 °C / 226.4 °F Method - No information available

Autoignition Temperature
Decomposition Temperature
PH
Viscosity

No data available
No data available
No data available
No data available

Water Solubility Decomposes in contact with water

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Vapor Pressure No data available

Density / Specific Gravity 1.137

Bulk DensityNot applicableLiquidVapor Density5.81(Air = 1.0)

Particle characteristics Not applicable (liquid)

9.2. Other information

Molecular FormulaC9 H9 Cl OMolecular Weight168.62

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SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

Yes

10.2. Chemical stability

Moisture sensitive.

10.3. Possibility of hazardous reactions

Hazardous Polymerization

Hazardous polymerization does not occur.

Hazardous Reactions

None under normal processing.

10.4. Conditions to avoid

Incompatible products. Excess heat. Exposure to moist air or water. Exposure to moisture.

10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO2). Hydrogen chloride gas.

SECTION 11: TOXICOLOGICAL INFORMATION

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

Product Information

(a) acute toxicity;

OralNo data availableDermalNo data availableInhalationCategory 3

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzenepropanoyl chloride	=	-	2750 mg/m³/4h (Rat)

(b) skin corrosion/irritation; Category 2

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

(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; No data available

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No data available (i) STOT-repeated exposure;

Target Organs None known.

No data available (j) aspiration hazard;

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

delayed

Symptoms / effects, both acute and Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated. Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation.

11.2. Information on other hazards

Assess endocrine disrupting properties for human health. This product does not contain any **Endocrine Disrupting Properties**

known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity **Ecotoxicity effects**

Do not empty into drains. Reacts with water so no ecotoxicity data for the substance is available. Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae
Benzenepropanoyl chloride			Desmodesmus subspicatus:
			EC50 = 56 mg/L (72 h)

12.2. Persistence and degradability No information available

Persistence Persistence is unlikely, based on information available.

Degradability Decomposes in contact with water.

Degradation in sewage No information available. Decomposes in contact with water. Contains substances known to

treatment plant be hazardous to the environment or not degradable in waste water treatment plants.

12.3. Bioaccumulative potential Product does not bioaccumulate due to reaction with water

12.4. Mobility in soil Decomposes in contact with water Is not likely mobile in the environment.

12.5. Results of PBT and vPvB Decomposes in contact with water. Substance is not considered persistent,

assessment 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 This product does not contain any known or suspected substance

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Ozone Depletion Potential 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.

According to the European Waste Catalog, Waste Codes are not product specific, but **European Waste Catalogue (EWC)**

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. Do not flush to sewer. Large amounts will affect pH

and harm aquatic organisms. Do not let this chemical enter the environment.

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 UN2810

14.2. UN proper shipping name TOXIC LIQUID, ORGANIC, N.O.S.

Technical Shipping Name Hydrocinnamoyl chloride

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

ADR

UN2810 14.1. UN number

14.2. UN proper shipping name TOXIC LIQUID, ORGANIC, N.O.S.

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Hydrocinnamoyl chloride **Technical Shipping Name**

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

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk Not applicable, packaged goods according to IMO instruments

SECTION 15: REGULATORY INFORMATION

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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
Benzenepropanoyl chloride	645-45-4	211-443-6	ī	-	ı	X	1	-	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Benzenepropanoyl chloride	645-45-4	Х	ACTIVE	-	X	Х	Х	Х

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

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)
Benzenepropanoyl chloride	645-45-4	-	-	-

Component	CAS No	Seveso III Directive (2012/18/EC) -	Seveso III Directive (2012/18/EC) -
		Qualifying Quantities for Major Accident	Qualifying Quantities for Safety Report
		Notification	Requirements
Benzenepropanoyl chloride	645-45-4	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 = 2 (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

H331 - Toxic if inhaled

H315 - Causes skin irritation

H412 - Harmful to aquatic life with long lasting effects

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.

Creation Date 20-Sep-2010 **Revision Date** 01-Sep-2023

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

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

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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