

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

1.1. Product identifier

Product Description: 3-Isocyanatobenzoyl chloride
Cat No. : L16002
Molecular Formula C8 H4 Cl 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

Thermo Fisher (Kandel) GmbH
Erlenbachweg 2, 76870 Kandel, Germany
Tel: +49 (0) 721 84007 280
Fax: +49 (0) 721 84007 300

Swiss distributor - Fisher Scientific AG
Neuhofstrasse 11, CH 4153 Reinach
Tel: +41 (0) 56 618 41 11
<https://www.fishersci.ch/ch/en/customer-help-support/forms/email-us.html>

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

CLP Classification - Regulation (EC) No 1272/2008

Physical hazards

SAFETY DATA SHEET

3-Isocyanatobenzoyl chloride

Revision Date 15-Mar-2024

Based on available data, the classification criteria are not met

Health hazards

Acute oral toxicity
Acute Inhalation Toxicity - Vapors
Skin Corrosion/Irritation
Serious Eye Damage/Eye Irritation
Skin Sensitization

Category 4 (H302)
Category 4 (H332)
Category 1 B (H314)
Category 1 (H318)
Category 1 (H317)

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

Danger

Hazard Statements

H314 - Causes severe skin burns and eye damage
H317 - May cause an allergic skin reaction
H302 + H332 - Harmful if swallowed or if inhaled

Precautionary Statements

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P301 + P330 + P331 - IF SWALLOWED: Rinse mouth. Do NOT induce vomiting
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P310 - Immediately call a POISON CENTER or doctor/physician
P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

2.3. Other hazards

Lachrymator (substance which increases the flow of tears)
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-Isocyanatobenzoyl chloride	5180-79-0		<=100	Acute Tox. 4 (H302) Acute Tox. 4 (H332) Skin Corr. 1B (H314) Eye Dam. 1 (H318)

SAFETY DATA SHEET

3-Isocyanatobenzoyl chloride

Revision Date 15-Mar-2024

				Skin Sens. 1 (H317)
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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. Immediate medical attention is required.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Call a physician immediately.
Ingestion	Do NOT induce vomiting. Clean mouth with water. Never give anything by mouth to an unconscious person. Call a physician immediately.
Inhalation	If not breathing, give artificial respiration. Remove from exposure, lie down. 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. Call a physician immediately.
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

Causes burns by all exposure routes. May cause allergic skin reaction. 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: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician	Treat symptomatically.
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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

No information available.

5.2. Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors. The product causes burns of eyes, skin and mucous membranes.

Hazardous Combustion Products

SAFETY DATA SHEET

3-Isocyanatobenzoyl chloride

Revision Date 15-Mar-2024

None under normal use conditions.

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. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

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

Soak up with inert absorbent material. 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. 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.

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

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

Storage Class/LGK 8A

Switzerland - Storage of hazardous substances

Storage class - SC 8
<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

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

SAFETY DATA SHEET

3-Isocyanatobenzoyl chloride

Revision Date 15-Mar-2024

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

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	See manufacturers	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
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.
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

SAFETY DATA SHEET

3-Isocyanatobenzoyl chloride

Revision Date 15-Mar-2024

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 141 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	Liquid	
Appearance	Light yellow	
Odor	pungent	
Odor Threshold	No data available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	91 °C / 195.8 °F	
Flammability (liquid)	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	> 110 °C / > 230 °F	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	1.333 g/cm3	@ 20 °C
Bulk Density	Not applicable	Liquid
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

9.2. Other information

Molecular Formula	C8 H4 Cl N O2
Molecular Weight	181.58

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity	None known, based on information available
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10.2. Chemical stability	Stable under normal conditions.
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10.3. Possibility of hazardous reactions

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

SAFETY DATA SHEET

3-Isocyanatobenzoyl chloride

Revision Date 15-Mar-2024

10.4. Conditions to avoid

Incompatible products. Excess heat.

10.5. Incompatible materials

None known.

10.6. Hazardous decomposition products

None under normal use conditions.

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	No data available
Inhalation	Category 4

(b) skin corrosion/irritation; Category 1 B

(c) serious eye damage/irritation; Category 1

(d) respiratory or skin sensitization;

Respiratory	No data available
Skin	Category 1

May cause sensitization by skin contact

(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

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

Symptoms / effects, both acute and delayed 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. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing.

11.2. Information on other hazards

SAFETY DATA SHEET

3-Isocyanatobenzoyl chloride

Revision Date 15-Mar-2024

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

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

12.2. Persistence and degradability No information available

12.3. Bioaccumulative potential No information available

12.4. Mobility in soil No information available

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 was used. Do not empty into drains. Do not flush to sewer. Large amounts will affect pH and harm aquatic organisms.

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

UN2922

SAFETY DATA SHEET

3-Isocyanatobenzoyl chloride

Revision Date 15-Mar-2024

14.2. UN proper shipping name	Corrosive liquid, toxic, n.o.s.
Technical Shipping Name	(3-isocyanatobenzoyl chloride)
14.3. Transport hazard class(es)	8
Subsidiary Hazard Class	6.1
14.4. Packing group	II

ADR

14.1. UN number	UN2922
14.2. UN proper shipping name	Corrosive liquid, toxic, n.o.s.
Technical Shipping Name	(3-isocyanatobenzoyl chloride)
14.3. Transport hazard class(es)	8
Subsidiary Hazard Class	6.1
14.4. Packing group	II

IATA

14.1. UN number	UN2922
14.2. UN proper shipping name	Corrosive liquid, toxic, n.o.s.
Technical Shipping Name	(3-isocyanatobenzoyl chloride)
14.3. Transport hazard class(es)	8
Subsidiary Hazard Class	6.1
14.4. Packing group	II

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
3-Isocyanatobenzoyl chloride	5180-79-0	-	-	-	-	X	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
3-Isocyanatobenzoyl chloride	5180-79-0	-	-	-	-	-	-	-

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	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
3-Isocyanatobenzoyl chloride	5180-79-0	-	-	-

Seveso III Directive (2012/18/EC)

SAFETY DATA SHEET

3-Isocyanatobenzoyl chloride

Revision Date 15-Mar-2024

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-Isocyanatobenzoyl chloride	5180-79-0	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 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

H302 - Harmful if swallowed

H332 - Harmful if inhaled

H314 - Causes severe skin burns and eye damage

H317 - May cause an allergic skin reaction

H318 - Causes serious eye damage

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical 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

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

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

SAFETY DATA SHEET

3-Isocyanatobenzoyl chloride

Revision Date 15-Mar-2024

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

Key literature references and sources for data

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

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

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)

Training Advice

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

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.

Prepared By

Health, Safety and Environmental Department

Revision Date

15-Mar-2024

Revision Summary

New emergency telephone response service provider.

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