

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

1.1. Product identifier

Product Description: **3,5-Bis(trifluoromethyl)benzaldehyde**
Cat No. : **307690000; 307690010; 307690050**
CAS No **401-95-6**
Molecular Formula **C9 H4 F6 O**

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 Pharmaceuticaaan 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

Acute oral toxicity
Skin Corrosion/Irritation

Category 4 (H302)
Category 2 (H315)

SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)benzaldehyde

Revision Date 29-Sep-2023

Serious Eye Damage/Eye Irritation
Specific target organ toxicity - (single exposure)

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
H302 - Harmful if swallowed
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation
Combustible liquid

Precautionary Statements

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

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 |
|--------------------------------------|----------|-------|----------|---|
| 3,5-Bis(trifluoromethyl)benzaldehyde | 401-95-6 | | 97 | STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 4 (H302) |

SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)benzaldehyde

Revision Date 29-Sep-2023

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

| | |
|---|--|
| 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 soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention. |
| Ingestion | Clean mouth with water. Get medical attention. |
| Inhalation | Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention. |
| 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

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

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. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

Combustible material. Containers may explode when heated.

Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO₂), Gaseous hydrogen fluoride (HF).

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

Remove all sources of ignition. Take precautionary measures against static discharges.

SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)benzaldehyde

Revision Date 29-Sep-2023

6.2. Environmental precautions

See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Do not let this chemical enter the environment. Remove all sources of ignition.

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

Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Keep away from open flames, hot surfaces and sources of ignition.

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. Keep away from heat, sparks and flame. Store under an inert atmosphere. Keep containers tightly closed in a dry, cool and well-ventilated place.

Technical Rules for Hazardous Substances (TRGS) 510 Class 10
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

SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)benzaldehyde

Revision Date 29-Sep-2023

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 | See manufacturers | - | EN 374 | (minimum requirement) |
| Neoprene | recommendations | | | |
| Natural rubber | | | | |
| PVC | | | | |

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

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

No protective equipment is needed under normal use conditions.

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

Small scale/Laboratory use

Maintain adequate ventilation

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

No information available

Odor Threshold

No data available

Melting Point/Range

No data available

Softening Point

No data available

SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)benzaldehyde

Revision Date 29-Sep-2023

| | | |
|---|--------------------------|-----------------------------------|
| Boiling Point/Range | 37 °C / 98.6 °F | @ 1.3 mmHg |
| Flammability (liquid) | Combustible liquid | On basis of test data |
| Flammability (solid,gas) | Not applicable | Liquid |
| Explosion Limits | No data available | |
| Flash Point | 69 °C / 156.2 °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 | 1.470 | |
| Bulk Density | Not applicable | Liquid |
| Vapor Density | No data available | (Air = 1.0) |
| Particle characteristics | Not applicable (liquid) | |

9.2. Other information

| | |
|----------------------|--|
| Molecular Formula | C9 H4 F6 O |
| Molecular Weight | 242.12 |
| Explosive Properties | explosive air/vapour mixtures possible |

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Stable under normal conditions. Air sensitive.

10.3. Possibility of hazardous reactions

| | |
|--------------------------|---------------------------|
| Hazardous Polymerization | No information available. |
| Hazardous Reactions | No information available. |

10.4. Conditions to avoid

Exposure to air. Incompatible products. Keep away from open flames, hot surfaces and sources of ignition.

10.5. Incompatible materials

Strong oxidizing agents. Strong acids. Strong bases. Strong reducing agents.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO₂). Gaseous hydrogen fluoride (HF).

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 |
|-----------------------------|------------|

SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)benzaldehyde

Revision Date 29-Sep-2023

| | |
|--|--|
| Dermal | No data available |
| Inhalation | No data available |
| (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 |
| Results / Target organs | Respiratory system. |
| (i) STOT-repeated exposure; | No data available |
| Target Organs | No information available. |
| (j) aspiration hazard; | No data available |
| Other Adverse Effects | The toxicological properties have not been fully investigated. |
| Symptoms / effects, both acute and delayed | Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting. |

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 | No information available |
| | Persistence is unlikely, based on information available. |

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)benzaldehyde

Revision Date 29-Sep-2023

12.4. Mobility in soil

The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Will likely be mobile in the environment due to its volatility. Disperses rapidly in air.

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.

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

SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)benzaldehyde

Revision Date 29-Sep-2023

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)

| Component | CAS No | EINECS | ELINCS | NLP | IECSC | TCSI | KECL | ENCS | ISHL |
|--------------------------------------|----------|--------|--------|-----|-------|------|------|------|------|
| 3,5-Bis(trifluoromethyl)benzaldehyde | 401-95-6 | - | - | - | - | X | - | - | X |

| Component | CAS No | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|--------------------------------------|----------|------|---|-----|------|------|-------|-------|
| 3,5-Bis(trifluoromethyl)benzaldehyde | 401-95-6 | - | - | - | - | - | - | - |

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) |
|--------------------------------------|----------|---|---|---|
| 3,5-Bis(trifluoromethyl)benzaldehyde | 401-95-6 | - | - | - |

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 |
|--------------------------------------|----------|---|--|
| 3,5-Bis(trifluoromethyl)benzaldehyde | 401-95-6 | 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)?

See table for values

| Component | OECD PFAS | US (EPA) PFAS | EU (ECHA) PFAS | UK (HSE) PFAS | Chemsec PFAS (Sin List) |
|--------------------------------------|-----------|---------------|----------------|---------------|-------------------------|
| 3,5-Bis(trifluoromethyl)benzaldehyde | - | - | Listed | Listed | - |

SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)benzaldehyde

Revision Date 29-Sep-2023

| | | | | | |
|-------------------|--|--|--|--|--|
| (CAS #: 401-95-6) | | | | | |
|-------------------|--|--|--|--|--|

PFAS Legend

Listed = Meets the PFAS definition of the named authority

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)

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

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

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

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)

SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)benzaldehyde

Revision Date 29-Sep-2023

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.

Revision Date 29-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