

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

1.1. Product identifier

Product Description: 6-Chloro-7-deazapurine
Cat No. : 437440000; 437440010; 437440050
Synonyms 4-Chloro-7H-pyrrolo[2,3-d]pyrimidine
CAS No 3680-69-1
EC No 628-079-2
Molecular Formula C6 H4 Cl N3

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

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Acute oral toxicity

Category 3 (H301)

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

H301 - Toxic if swallowed

Precautionary Statements

P264 - Wash face, hands and any exposed skin thoroughly after handling
P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting
P405 - Store locked up

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 |
|--|-----------|-----------|----------|---|
| 4-Chloro-7H-Pyrrolo [2,3-d] Pyrimidine | 3680-69-1 | 628-079-2 | >95 | Acute Tox. 3 (H301) |

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

In the case of contact with eyes, rinse immediately with plenty of water and seek medical

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advice.

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.

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, 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.

Hazardous Combustion Products

Thermal decomposition can lead to release of irritating gases and vapors, Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), 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. Avoid dust formation. 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.

6.3. Methods and material for containment and cleaning up

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Sweep up and shovel into suitable containers for disposal. Avoid dust formation.

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. Avoid dust formation. Use only under a chemical fume hood. Do not breathe (dust, vapor, mist, gas). 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 containers tightly closed in a dry, cool and well-ventilated place.

Technical Rules for Hazardous Substances (TRGS) 510 Class 6.1C
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

Predicted No Effect Concentration (PNEC)

No information available.

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8.2. Exposure controls

Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas.

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

Skin and body protection Long sleeved clothing.

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 compatibility, 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 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: Particulates filter conforming to EN 143

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:- 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

Physical State Solid

Appearance Tan

Odor No information available

Odor Threshold No data available

Melting Point/Range 180.9 - 182.5 °C / 357.6 - 360.5 °F

Softening Point No data available

Boiling Point/Range No information available

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| | | |
|---|--------------------------|-----------------------------------|
| Flammability (liquid) | Not applicable | Solid |
| Flammability (solid,gas) | No information available | |
| Explosion Limits | No data available | |
| Flash Point | No information available | Method - No information available |
| Autoignition Temperature | No data available | |
| Decomposition Temperature | No data available | |
| pH | No information available | |
| Viscosity | Not applicable | Solid |
| 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 | No data available | |
| Bulk Density | No data available | |
| Vapor Density | Not applicable | Solid |
| Particle characteristics | No data available | |

9.2. Other information

| | |
|-------------------|------------------------|
| Molecular Formula | C6 H4 Cl N3 |
| Molecular Weight | 153.57 |
| Evaporation Rate | Not applicable - Solid |

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 Polymerization | Hazardous polymerization does not occur. |
| Hazardous Reactions | None under normal processing. |

10.4. Conditions to avoid

Incompatible products. Excess heat. Avoid dust formation.

10.5. Incompatible materials

Strong oxidizing agents. Strong acids.

10.6. Hazardous decomposition products

Thermal decomposition can lead to release of irritating gases and vapors. Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NO_x). 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; | |
| Oral | Category 3 |
| Dermal | No data available |

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| | |
|--|--|
| Inhalation | No data available |
| (b) skin corrosion/irritation; | No data available |
| (c) serious eye damage/irritation; | No data available |
| (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; | No data available |
| (i) STOT-repeated exposure; | No data available |
| Target Organs | None known. |
| (j) aspiration hazard; | Not applicable Solid |
| Symptoms / effects, both acute and delayed | No information available. |

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

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

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| | |
|---|--|
| 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. |

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

| | |
|---|--|
| 14.1. UN number | UN2811 |
| 14.2. UN proper shipping name Technical Shipping Name | TOXIC SOLID, ORGANIC, N.O.S. 6-Chloro-7-deazapurine |
| 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 Technical Shipping Name | TOXIC SOLID, ORGANIC, N.O.S. 6-Chloro-7-deazapurine |
| 14.3. Transport hazard class(es) | 6.1 |
| 14.4. Packing group | III |

IATA

| | |
|---|--|
| 14.1. UN number | UN2811 |
| 14.2. UN proper shipping name Technical Shipping Name | TOXIC SOLID, ORGANIC, N.O.S. 6-Chloro-7-deazapurine |
| 14.3. Transport hazard class(es) | 6.1 |
| 14.4. Packing group | III |

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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 |
|--|-----------|--------|--------|-----|-------|------|------|------|------|
| 4-Chloro-7H-Pyrrolo [2,3-d] Pyrimidine | 3680-69-1 | - | - | - | - | X | - | - | X |

| Component | CAS No | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|--|-----------|------|---|-----|------|------|-------|-------|
| 4-Chloro-7H-Pyrrolo [2,3-d] Pyrimidine | 3680-69-1 | - | - | - | - | - | - | - |

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) |
|--|-----------|---|---|---|
| 4-Chloro-7H-Pyrrolo [2,3-d] Pyrimidine | 3680-69-1 | - | - | - |

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 |
|--|-----------|---|--|
| 4-Chloro-7H-Pyrrolo [2,3-d] Pyrimidine | 3680-69-1 | 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 .

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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

H301 - Toxic if swallowed

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

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

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

DSL/NDL - 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

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)

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.

Creation Date 28-Dec-2010

Revision Date 13-Oct-2023

Revision Summary Not applicable.

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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