



SAFETY DATA SHEET

Creation Date 29-Apr-2014

Revision Date

Revision Number 0

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

1.1. Product identifier

Product Description: 6,7-Dihydro-5H-pyrrolo[3,4-d]pyrimidine dihydrochloride, 95%
Cat No. : 454210000; 454212500; 454210010
CAS-No 157327-51-0
Molecular Formula C6 H9 Cl2 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 Acros Organics BVBA
Janssen Pharmaceuticaaan 3a
2440 Geel, Belgium
E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-ACROS-01 / **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 - Regulation (EC) No 1272/2008

Physical hazards

Based on available data, the classification criteria are not met

Health hazards

Acute oral toxicity	Category 4
Skin Corrosion/irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3

Environmental hazards

Based on available data, the classification criteria are not met

Classification according to EU Directives 67/548/EEC or 1999/45/EC

Symbol(s) Xn - Harmful
R-phrases(s) R22 - Harmful if swallowed
R36/37/38 - Irritating to eyes, respiratory system and skin

For the full text of the R-phrases and H-Statements mentioned in this Section, see Section 16

2.2. Label elements

**Signal Word****Warning****Hazard Statements**

H302 - Harmful if swallowed
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation

Precautionary Statements

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P304 + P340 - IF INHALED: Remove to fresh air and keep at rest in a position comfortable for breathing
P312 - Call a POISON CENTER or doctor/ physician if you feel unwell
P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection

2.3. Other hazards

No information available

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS-No	EC-No.	Weight %	CLP Classification - Regulation (EC) No 1272/2008	DSD Classification - 67/548/EEC
6,7-Dihydro-5H-pyrrolo[3,4-d]pyrimidine dihydrochloride	157327-51-0		>=95	Acute Tox. 4 (H302) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) STOT SE 3 (H335)	Xn;R22 Xi;R36/37/38

For the full text of the R-phrases and H-Statements mentioned in this Section, 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. Obtain medical attention.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. Get medical attention if symptoms occur..

Ingestion

Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.

Inhalation

Move to fresh air. If breathing is difficult, give oxygen. Get medical attention immediately if symptoms occur.

Protection of First-aiders

Use personal protective equipment.

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**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

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.

SECTION 6: ACCIDENTAL RELEASE MEASURES**6.1. Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Ensure adequate ventilation. Avoid dust formation.

6.2. Environmental precautions

Should not be released into the environment.

6.3. Methods and material for containment and cleaning up

Sweep up or vacuum up spillage and collect in suitable container 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. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

7.2. Conditions for safe storage, including any incompatibilities

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

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.

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) No information available.

<u>Route of exposure</u>	Acute effects (local)	Acute effects (systemic)	Chronic effects (local)	Chronic effects (systemic)
Oral				
Dermal				
Inhalation				

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
Natural rubber	See manufacturers	-	EN 374	(minimum requirement)
Nitrile rubber	recommendations			
Neoprene				
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.

6,7-Dihydro-5H-pyrrolo[3,4-d]pyrimidine dihydrochloride, 95%

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.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.
Environmental exposure controls	No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Appearance	Brown	
Physical State	Solid.	
Odor	No information available	
Odor Threshold	No data available	
pH	No information available.	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	No information available	
Flash Point	No information available.	Method - No information available
Evaporation Rate	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available.	
Vapor Pressure	No data available	
Vapor Density	Not applicable	Solid
Specific Gravity / Density	No data available	
Bulk Density	No data available	
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	Not applicable	
Decomposition temperature	No data available	
Viscosity	Not applicable	Solid
Explosive Properties	No information available	
Oxidizing Properties	No information available	

9.2. Other information

Molecular Formula	C6 H9 Cl2 N3
Molecular Weight	194.06

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity	None known, based on information available
10.2. Chemical stability	Stable under normal conditions.

6,7-Dihydro-5H-pyrrolo[3,4-d]pyrimidine dihydrochloride, 95%

10.3. Possibility of hazardous reactions**Hazardous Polymerization
Hazardous Reactions**Hazardous polymerization does not occur.
None under normal processing.**10.4. Conditions to avoid**

Incompatible products, Excess heat, Exposure to light, Avoid dust formation.

10.5. Incompatible materials

Strong oxidizing agents. Strong acids.

10.6. Hazardous decomposition productsCarbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), Hydrogen chloride gas.**SECTION 11: TOXICOLOGICAL INFORMATION****11.1. Information on toxicological effects****Product Information****(a) acute toxicity;**

Oral	Category 4
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

(i) STOT-repeated exposure;

No data available

Target Organs

No information available

(j) aspiration hazard;Not applicable
Solid**Symptoms / effects,
both acute and delayed**

No information available

SECTION 12: ECOLOGICAL INFORMATION**12.1. Toxicity**

6,7-Dihydro-5H-pyrrolo[3,4-d]pyrimidine dihydrochloride, 95%

SECTION 12: ECOLOGICAL INFORMATION

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. Other adverse effects	
Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant	This product does not contain any known or suspected substance
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..
European Waste Catalogue (EWC)	According to the European Waste Catalogue, 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	
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. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION**15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture****International Inventories**

X = listed

National Regulations

Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

Take note of Dir 94/33/EC on the protection of young people at work

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

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION**Full text of R-phrases referred to under sections 2 and 3**

R22 - Harmful if swallowed

R36/37/38 - Irritating to eyes, respiratory system and skin

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**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**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**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**PNEC** - Predicted No Effect Concentration**LD50** - Lethal Dose 50%**EC50** - Effective Concentration 50%**POW** - Partition coefficient Octanol:Water**vPvB** - very Persistent, very Bioaccumulative**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 Compounds**Key literature references and sources for data**

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 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 29-Apr-2014

Revision Date

Revision Summary Initial Release.

This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006

Disclaimer

The information provided on 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 guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as 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 material or in any process, unless specified in the text.

End of Safety Data Sheet