

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/21/2020

Revision date 09/21/2020

1 Identification

- **Product identifier**
- **Trade name:** PLX51107
- **Synonym**
4-[6-(3,5-dimethyl-4-isoxazolyl)-1-[(1S)-1-(2-pyridinyl)ethyl]-1H-pyrrolo[3,2-b]pyridin-3-yl]-benzoic acid
- **Article number:** 30742
- **CAS Number:**
1627929-55-8
- **Application of the substance / the mixture** For research use only, not for human or veterinary use.
- **Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**
Cayman Chemical Co.
1180 E. Ellsworth Rd.
Ann Arbor, MI 48108
USA
- **Information department:** Product safety department
- **Emergency telephone number:**
During normal opening times: +1 (734) 971-3335
US/CANADA: 800-424-9300
Outside US/CANADA: 703-741-5970

2 Hazard(s) identification

- **Classification of the substance or mixture**



GHS07

Acute Tox. 4 H302 Harmful if swallowed.
Skin Irrit. 2 H315 Causes skin irritation.
Eye Irrit. 2A H319 Causes serious eye irritation.
STOT SE 3 H335 May cause respiratory irritation.

- **Label elements**

- **GHS label elements**

The substance is classified and labeled according to the Globally Harmonized System (GHS).

- **Hazard pictograms**



GHS07

- **Signal word** Warning

- **Hazard statements**

Harmful if swallowed.
Causes skin irritation.
Causes serious eye irritation.
May cause respiratory irritation.

(Contd. on page 2)

US

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/21/2020

Revision date 09/21/2020

Trade name: PLX51107

(Contd. from page 1)

Precautionary statements

Avoid breathing dust/fume/gas/mist/vapors/spray
 Wash thoroughly after handling.
 Do not eat, drink or smoke when using this product.
 Use only outdoors or in a well-ventilated area.
 Wear protective gloves / eye protection / face protection.
 If swallowed: Call a poison center/doctor if you feel unwell.
 Rinse mouth.
 If on skin: Wash with plenty of water.
 Specific treatment (see on this label).
 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
 If skin irritation occurs: Get medical advice/attention.
 Take off contaminated clothing and wash it before reuse.
 If eye irritation persists: Get medical advice/attention.
 Store in a well-ventilated place. Keep container tightly closed.
 Store locked up.
 Dispose of contents/container in accordance with local/regional/national/international regulations.

Classification system:

NFPA ratings (scale 0 - 4)



HMIS-ratings (scale 0 - 4)



Other hazards

Results of PBT and vPvB assessment

- **PBT:** Not applicable.
- **vPvB:** Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances

CAS No. Description

1627929-55-8 PLX51107

4 First-aid measures

Description of first aid measures

General information:

Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.

• **After inhalation:** In case of unconsciousness place patient stably in side position for transportation.

• **After skin contact:** Immediately wash with water and soap and rinse thoroughly.

After eye contact:

Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.

(Contd. on page 3)

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/21/2020

Revision date 09/21/2020

Trade name: PLX51107

(Contd. from page 2)

- **After swallowing:** Immediately call a doctor.
- **Information for doctor:**
- **Most important symptoms and effects, both acute and delayed**
May cause anemia, cough, CNS depression, drowsiness, headache, heart damage, lassitude (weakness, exhaustion), liver damage, narcosis, reproductive effects, teratogenic effects.
No further relevant information available.
- **Indication of any immediate medical attention and special treatment needed**
No further relevant information available.

5 Fire-fighting measures

- **Extinguishing media**
- **Suitable extinguishing agents:**
Use fire fighting measures that suit the environment.
A solid water stream may be inefficient.
- **Special hazards arising from the substance or mixture** No further relevant information available.
- **Advice for firefighters**
- **Protective equipment:** No special measures required.

6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures** Not required.
- **Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:** Ensure adequate ventilation.
- **Reference to other sections**
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.
- **Protective Action Criteria for Chemicals**
- **PAC-1:** Substance is not listed.
- **PAC-2:** Substance is not listed.
- **PAC-3:** Substance is not listed.

7 Handling and storage

- **Handling:**
- **Precautions for safe handling**
No special precautions are necessary if used correctly.
Avoid breathing dust/fume/gas/mist/vapours/spray.
Avoid prolonged or repeated exposure.
Keep away from sources of ignition.
Take precautionary measures against static discharge.re.
- **Information about protection against explosions and fires:** No special measures required.
- **Conditions for safe storage, including any incompatibilities**
Keep container tightly closed.
Store in accordance with information listed on the product insert.
- **Storage:**
- **Requirements to be met by storerooms and receptacles:** No special requirements.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:** Keep receptacle tightly sealed.

(Contd. on page 4)

-US-

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/21/2020

Revision date 09/21/2020

Trade name: PLX51107

(Contd. from page 3)

- **Specific end use(s)** No further relevant information available.

8 Exposure controls/personal protection

- **Additional information about design of technical systems:** No further data; see item 7.
- **Control parameters**
- **Components with limit values that require monitoring at the workplace:**
The following constituent is the only constituent of the product which has a PEL, TLV or other recommended exposure limit.
The following constituents are the only constituents of the product which have a PEL, TLV or other recommended exposure limit.
At this time, the remaining constituent has no known exposure limits.
At this time, the other constituents have no known exposure limits.
- **Additional information:** The lists that were valid during the creation were used as basis.
- **Exposure controls**
- **Personal protective equipment:**
- **General protective and hygienic measures:**
Keep away from foodstuffs, beverages and feed.
Immediately remove all soiled and contaminated clothing.
Wash hands before breaks and at the end of work.
Avoid contact with the eyes and skin.
- **Breathing equipment:**
In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.
- **Protection of hands:**



Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation. Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture. Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

- **Material of gloves**
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.
- **Penetration time of glove material**
The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.
- **Eye protection:**



Tightly sealed goggles

US

(Contd. on page 5)

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/21/2020

Revision date 09/21/2020

Trade name: PLX51107

(Contd. from page 4)

9 Physical and chemical properties

· Information on basic physical and chemical properties

· General Information

· Appearance:

Form: Solid
Color: Not determined.

· Odor: Characteristic

· Structural Formula C₂₆H₂₂N₄O₃

· Molecular Weight 438.5 g/mol

· Odor threshold: Not determined.

· pH-value: Not applicable.

· Change in condition

Melting point/Melting range: Undetermined.

Boiling point/Boiling range: Undetermined.

· Flash point: Not applicable.

· Flammability (solid, gaseous): Product is not flammable.

· Decomposition temperature: Not determined.

· Auto igniting: Not determined.

· Danger of explosion: Product does not present an explosion hazard.

· Explosion limits:

Lower: Not determined.

Upper: Not determined.

· Vapor pressure: Not applicable.

· Density: Not determined.

· Relative density: Not determined.

· Vapor density: Not applicable.

· Evaporation rate: Not applicable.

· Solubility in / Miscibility with

Water: Not determined.

· Partition coefficient (n-octanol/water): Not determined.

· Viscosity:

Dynamic: Not applicable.

Kinematic: Not applicable.

SOLUBILITY ~50 mg/ml in DMSO

· Other information: No further relevant information available.

10 Stability and reactivity

· Reactivity: No further relevant information available.

· Chemical stability

· Thermal decomposition / conditions to be avoided:

No decomposition if used according to specifications.

· Possibility of hazardous reactions: No dangerous reactions known.

· Conditions to avoid: No further relevant information available.

· Incompatible materials: No further relevant information available.

(Contd. on page 6)

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/21/2020

Revision date 09/21/2020

Trade name: PLX51107

· **Hazardous decomposition products:** carbon oxides, nitrogen oxides

(Contd. from page 5)

11 Toxicological information

- **Information on toxicological effects**
- **Acute toxicity:**
- **Primary irritant effect:**
 - **on the skin:** Irritant to skin and mucous membranes.
 - **on the eye:** Irritating effect.
- **Sensitization:** No sensitizing effects known.
- **Additional toxicological information:**
- **Carcinogenic categories**
- **IARC (International Agency for Research on Cancer)** Substance is not listed.
- **NTP (National Toxicology Program)** Substance is not listed.
- **OSHA-Ca (Occupational Safety & Health Administration)** Substance is not listed.

12 Ecological information

- **Toxicity**
- **Aquatic toxicity:** No further relevant information available.
- **Persistence and degradability** No further relevant information available.
- **Behavior in environmental systems:**
- **Bioaccumulative potential** No further relevant information available.
- **Mobility in soil** No further relevant information available.
- **Additional ecological information:**
- **General notes:**

Water hazard class 1 (Self-assessment): slightly hazardous for water
Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.
- **Other adverse effects** No further relevant information available.

13 Disposal considerations

- **Waste treatment methods**
- **Recommendation:**

Must not be disposed of together with household garbage. Do not allow product to reach sewage system.
- **Uncleaned packagings:**
- **Recommendation:** Disposal must be made according to official regulations.

14 Transport information

- **UN-Number**
- **DOT, IMDG, IATA** not regulated

(Contd. on page 7)

US

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/21/2020

Revision date 09/21/2020

Trade name: PLX51107

(Contd. from page 6)

· UN proper shipping name	
· DOT, IMDG, IATA	not regulated
· Transport hazard class(es)	
· DOT, ADN, IMDG, IATA	
· Class	not regulated
· Packing group	
· DOT, IMDG, IATA	not regulated
· Environmental hazards:	Not applicable.
· Special precautions for user	Not applicable.
· Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
· UN "Model Regulation":	not regulated

15 Regulatory information

- **Safety, health and environmental regulations/legislation specific for the substance or mixture**
- **Sara**
- **Section 355 (extremely hazardous substances):** Substance is not listed.
- **Section 313 (Specific toxic chemical listings):** Substance is not listed.
- **TSCA (Toxic Substances Control Act):** Substance is not listed.
- **Hazardous Air Pollutants** Substance is not listed.
- **Proposition 65**
- **Chemicals known to cause cancer:** Substance is not listed.
- **Chemicals known to cause reproductive toxicity for females:** Substance is not listed.
- **Chemicals known to cause reproductive toxicity for males:** Substance is not listed.
- **Chemicals known to cause developmental toxicity:** Substance is not listed.
- **Carcinogenic categories**
- **EPA (Environmental Protection Agency)** Substance is not listed.
- **TLV (Threshold Limit Value established by ACGIH)** Substance is not listed.
- **NIOSH-Ca (National Institute for Occupational Safety and Health)** Substance is not listed.
- **GHS label elements**
The substance is classified and labeled according to the Globally Harmonized System (GHS).
- **Hazard pictograms**



GHS07

- **Signal word** Warning
- **Hazard statements**
Harmful if swallowed.
Causes skin irritation.
Causes serious eye irritation.
May cause respiratory irritation.
- **Precautionary statements**
Avoid breathing dust/fume/gas/mist/vapors/spray

(Contd. on page 8)

US

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/21/2020

Revision date 09/21/2020

Trade name: PLX51107

(Contd. from page 7)

Wash thoroughly after handling.
 Do not eat, drink or smoke when using this product.
 Use only outdoors or in a well-ventilated area.
 Wear protective gloves / eye protection / face protection.
 If swallowed: Call a poison center/doctor if you feel unwell.
 Rinse mouth.
 If on skin: Wash with plenty of water.
 Specific treatment (see on this label).
 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
 If skin irritation occurs: Get medical advice/attention.
 Take off contaminated clothing and wash it before reuse.
 If eye irritation persists: Get medical advice/attention.
 Store in a well-ventilated place. Keep container tightly closed.
 Store locked up.
 Dispose of contents/container in accordance with local/regional/national/international regulations.

- **Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

16 Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

- **Department issuing SDS:** Environment protection department.
- **Contact:** -
- **Date of preparation / last revision** 09/21/2020 / -
- **Abbreviations and acronyms:**
 IMDG: International Maritime Code for Dangerous Goods
 DOT: US Department of Transportation
 IATA: International Air Transport Association
 ACGIH: American Conference of Governmental Industrial Hygienists
 CAS: Chemical Abstracts Service (division of the American Chemical Society)
 NFPA: National Fire Protection Association (USA)
 HMIS: Hazardous Materials Identification System (USA)
 PBT: Persistent, Bioaccumulative and Toxic
 vPvB: very Persistent and very Bioaccumulative
 NIOSH: National Institute for Occupational Safety
 OSHA: Occupational Safety & Health
 TLV: Threshold Limit Value
 PEL: Permissible Exposure Limit
 REL: Recommended Exposure Limit
 Acute Tox. 4: Acute toxicity – Category 4
 Skin Irrit. 2: Skin corrosion/irritation – Category 2
 Eye Irrit. 2A: Serious eye damage/eye irritation – Category 2A
 STOT SE 3: Specific target organ toxicity (single exposure) – Category 3
- *** Data compared to the previous version altered.**

US