

Safety Data Sheet

acc. to OSHA HCS

Printing date 03/25/2020

Revision date 03/25/2020

1 Identification

- **Product identifier**
- **Trade name:** PF-05105679
- **Synonym** 3-[[[(1R)-1-(4-fluorophenyl)ethyl](3-quinolinylcarbonyl)amino]methyl]-benzoic acid
- **Article number:** 29489
- **CAS Number:**
1398583-31-7
- **EC number:**
809-223-5
- **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**



Acute Tox. 4 H302 Harmful if swallowed.

- **Label elements**
- **GHS label elements** The substance is classified and labeled according to the Globally Harmonized System (GHS).
- **Hazard pictograms**



- **Signal word** Warning
- **Hazard statements**
Harmful if swallowed.
- **Precautionary statements**
Wash thoroughly after handling.
Do not eat, drink or smoke when using this product.
If swallowed: Call a poison center/doctor if you feel unwell.
Rinse mouth.
Dispose of contents/container in accordance with local/regional/national/international regulations.

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- **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**
1398583-31-7 PF-05105679
- **Identification number(s)**
- **EC number:** 809-223-5

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:** Supply fresh air; consult doctor in case of complaints.
- **After skin contact:** Generally the product does not irritate the skin.
- **After eye contact:** Rinse opened eye for several minutes under running water.
- **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**

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- **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:** Pick up mechanically.
- **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**
 - Np special precautions are necessary if used correctly.
 - Avoid breathing dust/fume/gas/mist/vapours/spray.
 - Avoid prolonged or repeated exposure.
 - **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:** None.
 - **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:** Wash hands before breaks and at the end of work.
 - **Breathing equipment:** Not required.

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- **Protection of hands:**

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:** Not required.

9 Physical and chemical properties

- **Information on basic physical and chemical properties**

- **General Information**

- **Appearance:**

Form:	Solid
Color:	Not determined.
Odor:	Characteristic
Structural Formula	C ₂₆ H ₂₁ FN ₂ O ₃
Molecular Weight	428.5
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.

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Kinematic:	Not applicable.
SOLUBILITY	~10 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:** strong oxidizing agents
- **Hazardous decomposition products:** carbon oxides, hydrogen fluoride, nitrogen oxides

11 Toxicological information

- **Information on toxicological effects**
- **Acute toxicity:**
- **Primary irritant effect:**
- **on the skin:** No irritant effect.
- **on the eye:** No 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.

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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 |
| · 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).

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- **Hazard pictograms**



GHS07

- **Signal word** Warning

- **Hazard statements**

Harmful if swallowed.

- **Precautionary statements**

Wash thoroughly after handling.

Do not eat, drink or smoke when using this product.

If swallowed: Call a poison center/doctor if you feel unwell.

Rinse mouth.

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** 03/25/2020 / -

- **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

EINECS: European Inventory of Existing Commercial Chemical Substances

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

- *** Data compared to the previous version altered.**