

## Safety Data Sheet

acc. to OSHA HCS

Printing date 02/14/2021

Revision date 02/14/2021

### 1 Identification

- **Product identifier**
- **Trade name:** PA-824
- **Synonym**  
(6S)-6,7-dihydro-2-nitro-6-[[4-(trifluoromethoxy)phenyl]methoxy]-5H-imidazo[2,1-b][1,3]oxazine  
(S)-PA-824
- **Article number:** 13142
- **CAS Number:**  
187235-37-6
- **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

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**

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

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## Precautionary statements

Avoid breathing dust/fume/gas/mist/vapors/spray  
 Wash thoroughly after handling.  
 Use only outdoors or in a well-ventilated area.  
 Wear protective gloves / eye protection / face protection.  
 If on skin: Wash with plenty of water.  
 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.  
 Call a poison center/doctor if you feel unwell.  
 Specific treatment (see on this label).  
 Take off contaminated clothing and wash it before reuse.  
 If skin irritation occurs: Get medical advice/attention.  
 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)



Health = 2  
 Fire = 0  
 Reactivity = 0

### HMIS-ratings (scale 0 - 4)



Health = 2  
 Fire = 0  
 Reactivity = 0

### 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  
187235-37-6 PA-824

## 4 First-aid measures

### Description of first aid measures

- 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.
- After swallowing:** If symptoms persist consult 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.

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- **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.
- **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.

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- **Control parameters**
- **Components with limit values that require monitoring at the workplace:** Not required.
- **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

## 9 Physical and chemical properties

- **Information on basic physical and chemical properties**
- **General Information**
- **Appearance:**

<b>Form:</b>	Crystalline
<b>Color:</b>	Not determined.
- **Odor:** Characteristic
- **Structural Formula** C<sub>14</sub>H<sub>12</sub>F<sub>3</sub>N<sub>3</sub>O<sub>5</sub>
- **Molecular Weight** 359.3 g/mol
- **Odor threshold:** Not determined.
- **pH-value:** Not applicable.
- **Change in condition**
- **Melting point/Melting range:** Undetermined.

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<b>Boiling point/Boiling range:</b>	Undetermined.
· <b>Flash point:</b>	Not applicable.
· <b>Flammability (solid, gaseous):</b>	Product is not flammable.
· <b>Decomposition temperature:</b>	Not determined.
· <b>Auto igniting:</b>	Not determined.
· <b>Danger of explosion:</b>	Product does not present an explosion hazard.
· <b>Explosion limits:</b>	
<b>Lower:</b>	Not determined.
<b>Upper:</b>	Not determined.
· <b>Vapor pressure:</b>	Not applicable.
· <b>Density:</b>	Not determined.
· <b>Relative density</b>	Not determined.
· <b>Vapor density</b>	Not applicable.
· <b>Evaporation rate</b>	Not applicable.
· <b>Solubility in / Miscibility with Water:</b>	Not determined.
· <b>Partition coefficient (n-octanol/water):</b>	Not determined.
· <b>Viscosity:</b>	
<b>Dynamic:</b>	Not applicable.
<b>Kinematic:</b>	Not applicable.
<b>SOLUBILITY</b>	~0.33 mg/ml in a 1:2 solution of DMSO:PBS (pH 7.2); ~5 mg/ml in EtOH; ~33 mg/ml in DMSO & DMF
· <b>Other information</b>	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:** Irritant to skin and mucous membranes.
- **on the eye:** Irritating effect.
- **Sensitization:** No sensitizing effects known.

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- **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

· <b>UN-Number</b>	
· <b>DOT, IMDG, IATA</b>	not regulated
· <b>UN proper shipping name</b>	
· <b>DOT, IMDG, IATA</b>	not regulated
· <b>Transport hazard class(es)</b>	
· <b>DOT, ADN, IMDG, IATA</b>	
· <b>Class</b>	not regulated
· <b>Packing group</b>	
· <b>DOT, IMDG, IATA</b>	not regulated
· <b>Environmental hazards:</b>	Not applicable.

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- |  |                 |
|--|-----------------|
| · <b>Special precautions for user</b>  | Not applicable. |
| · <b>Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</b> | Not applicable. |
| · <b>UN "Model Regulation":</b>  | not regulated   |

### 15 Regulatory information

- **Safety, health and environmental regulations/legislation specific for the substance or mixture**  
No further relevant information available.
- **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.
- **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** 02/14/2021 / -
- **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  
 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