

## Safety Data Sheet

acc. to OSHA HCS

Printing date 03/28/2020

Revision date 03/28/2020

### 1 Identification

- **Product identifier**
- **Trade name:** 2-[3-(2,4-difluorophenyl)-4,5-dihydro-5-isoxazolyl]-1-(4-morpholinyl)-ethanone
- **Synonym** CPSI-1306
- **Article number:** 29905
- **CAS Number:**  
1309793-47-2
- **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**



Skin Irrit. 2 H315 Causes skin irritation.  
Eye Irrit. 2A H319 Causes serious eye irritation.  
Skin Sens. 1 H317 May cause an allergic skin reaction.  
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**



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

(Contd. on page 2)

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(Contd. from page 1)

Wash thoroughly after handling.  
 Use only outdoors or in a well-ventilated area.  
 Contaminated work clothing must not be allowed out of the workplace.  
 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 or rash occurs: Get medical advice/attention.  
 If eye irritation persists: Get medical advice/attention.  
 Wash contaminated clothing before reuse.  
 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**

1309793-47-2 2-[3-(2,4-difluorophenyl)-4,5-dihydro-5-isoxazolyl]-1-(4-morpholinyl)-ethanone

## 4 First-aid measures

· **Description of first aid measures**

· **After inhalation:**

Supply fresh air and to be sure call for a doctor.

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.

(Contd. on page 3)

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(Contd. from page 2)

- **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.
- **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.

US

(Contd. on page 4)

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(Contd. from page 3)

## 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

## 9 Physical and chemical properties

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

<b>Form:</b>	Crystalline
<b>Color:</b>	Not determined.

(Contd. on page 5)

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(Contd. from page 4)

· <b>Odor:</b>	Characteristic
· <b>Structural Formula</b>	C <sub>15</sub> H <sub>16</sub> F <sub>2</sub> N <sub>2</sub> O <sub>3</sub>
· <b>Molecular Weight</b>	310.3
· <b>Odor threshold:</b>	Not determined.
· <b>pH-value:</b>	Not applicable.
· <b>Change in condition</b>	
Melting point/Melting range:	Undetermined.
Boiling point/Boiling range:	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>	
Lower:	Not determined.
Upper:	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>	
Dynamic:	Not applicable.
Kinematic:	Not applicable.
<b>SOLUBILITY</b>	~0.2 mg/ml in a 1:4 solution of DMSO:PBS (pH 7.2); ~30 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:** No further relevant information available.
- **Hazardous decomposition products:** No dangerous decomposition products known.

US

(Contd. on page 6)

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(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:** Sensitization possible through skin contact.
- **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 |

(Contd. on page 7)

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(Contd. from page 6)

- |   |                 |
|---|-----------------|
| · <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. |
| · <b>Special precautions for user</b>   | Not applicable. |
| · <b>Transport in bulk according to Annex II of MARPOL 73/78 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**
- **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**
  - Causes skin irritation.
  - Causes serious eye irritation.
  - May cause an allergic skin reaction.
  - May cause respiratory irritation.
- **Precautionary statements**
  - Avoid breathing dust/fume/gas/mist/vapors/spray
  - Wash thoroughly after handling.
  - Use only outdoors or in a well-ventilated area.
  - Contaminated work clothing must not be allowed out of the workplace.
  - Wear protective gloves / eye protection / face protection.

(Contd. on page 8)



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*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 or rash occurs: Get medical advice/attention.*

*If eye irritation persists: Get medical advice/attention.*

*Wash contaminated clothing before reuse.*

*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** 03/28/2020 / -

· **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

Skin Irrit. 2: Skin corrosion/irritation – Category 2

Eye Irrit. 2A: Serious eye damage/eye irritation – Category 2A

Skin Sens. 1: Skin sensitisation – Category 1

STOT SE 3: Specific target organ toxicity (single exposure) – Category 3