



Safety Data Sheet

acc. to OSHA HCS

Printing date 07/21/2022

Revision date 07/21/2022

1 Identification

- **Product identifier**
- **Trade name:** Simeprevir (sodium salt)
- **Article number:** 22144
- **CAS Number:**
1241946-89-3
- **Application of the substance / the mixture**
This product is for research use - Not for human or veterinary diagnostic or therapeutic 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**



GHS08 Health hazard

Resp. Sens. 1 H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.
Muta. 2 H341 Suspected of causing genetic defects.
Repr. 2 H361 Suspected of damaging fertility or the unborn child.
STOT SE 1 H370 Causes damage to organs.



GHS05 Corrosion

Eye Dam. 1 H318 Causes serious eye damage.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

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Skin Irrit. 2 H315 Causes skin irritation.
 Skin Sens. 1 H317 May cause an allergic skin reaction.
 STOT SE 3 H335 May cause respiratory irritation.
 Aquatic Chronic 4 H413 May cause long lasting harmful effects to aquatic life.

· **Label elements**

· **GHS label elements**

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

· **Hazard pictograms**



GHS05 GHS07 GHS08

· **Signal word** Danger

· **Hazard statements**

H302 Harmful if swallowed.
 H315 Causes skin irritation.
 H318 Causes serious eye damage.
 H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.
 H317 May cause an allergic skin reaction.
 H341 Suspected of causing genetic defects.
 H361 Suspected of damaging fertility or the unborn child.
 H370 Causes damage to organs.
 H335 May cause respiratory irritation.
 H413 May cause long lasting harmful effects to aquatic life.

· **Precautionary statements**

P201 Obtain special instructions before use.
 P202 Do not handle until all safety precautions have been read and understood.
 P260 Do not breathe dust/fume/gas/mist/vapors/spray.
 P264 Wash thoroughly after handling.
 P270 Do not eat, drink or smoke when using this product.
 P272 Contaminated work clothing must not be allowed out of the workplace.
 P273 Avoid release to the environment.
 P280 Wear protective gloves/protective clothing/eye protection/face protection.
 P284 [In case of inadequate ventilation] wear respiratory protection.
 P301+P312 If swallowed: Call a poison center/doctor if you feel unwell.
 P302+P352 If on skin: Wash with plenty of water.
 P304+P341 If inhaled: If breathing is difficult, remove person to fresh air and keep comfortable for breathing.
 P305+P351+P338 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
 P310 Immediately call a poison center/doctor.
 P308+P313 IF exposed or concerned: Get medical advice/attention.
 P321 Specific treatment (see on this label).
 P330 Rinse mouth.
 P362+P364 Take off contaminated clothing and wash it before reuse.
 P333+P313 If skin irritation or rash occurs: Get medical advice/attention.
 P342+P311 If experiencing respiratory symptoms: Call a poison center/doctor.
 P363 Wash contaminated clothing before reuse.
 P405 Store locked up.
 P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

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- **Classification system:**
- **NFPA ratings (scale 0 - 4)**



Health = 3
Fire = 0
Reactivity = 0

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



Health = *3
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**
1241946-89-3 Simeprevir (sodium salt)

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 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. Then consult a doctor.
- **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.

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- **Advice for firefighters**
- **Protective equipment:** No special measures required.

6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures**
Wear protective equipment. Keep unprotected persons away.
- **Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:**
Use neutralizing agent.
Dispose contaminated material as waste according to item 13.
- **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**
Thorough dedusting.
Ensure good ventilation/exhaustion at the workplace.
- **Information about protection against explosions and fires:** No special measures required.
- **Conditions for safe storage, including any incompatibilities**
- **Storage:** Store in accordance with information listed on the product insert.
- **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.
- **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 skin.
Avoid contact with the eyes and skin.

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- **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:**

Form: Solid
Color: Not determined.

- **Odor:** Characteristic

- **Structural Formula** C₃₈H₄₇N₅O₇S₂ • XNa

- **Molecular Weight** 749.9 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.

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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	DMF: 30 mg/ml; DMSO: 30 mg/ml; DMSO:PBS (pH 7.2) (1:2): 0.33 mg/ml; Ethanol: slightly soluble
· 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 dioxide, carbon monoxide, hydrogen sulfide, 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:** Strong irritant with the danger of severe eye injury.
- **Sensitization:**
Sensitization possible through inhalation.
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.

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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 3 (Self-assessment): extremely hazardous for water
Do not allow product to reach ground water, water course or sewage system, even in small quantities.
Must not reach bodies of water or drainage ditch undiluted or unneutralized.
Danger to drinking water if even extremely small quantities leak into the ground.
- **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 |
| · 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 |

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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)** 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

All chemicals may pose unknown hazards and should be used with caution. This SDS applies only to the material as packaged. If this product is combined with other materials, deteriorates, or becomes contaminated, it may pose hazards not mentioned in this SDS. Cayman Chemical Company assumes no responsibility for incidental or consequential damages, including lost profits, arising from the use of these data. It shall be the user's responsibility to develop proper methods of handling and personal protection based on the actual conditions of use. While this SDS is based on technical data judged to be reliable, Cayman Chemical Company assumes no responsibility for the completeness or accuracy of the information contained herein.

- **Department issuing SDS:** Environment protection department.
- **Contact:** -
- **Date of preparation / last revision** 07/21/2022 / -
- **Abbreviations and acronyms:**
 IMDG: International Maritime Code for Dangerous Goods
 DOT: US Department of Transportation
 IATA: International Air Transport Association
 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 Dam. 1: Serious eye damage/eye irritation – Category 1
 Resp. Sens. 1: Respiratory sensitisation – Category 1
 Skin Sens. 1: Skin sensitisation – Category 1
 Muta. 2: Germ cell mutagenicity – Category 2
 Repr. 2: Reproductive toxicity – Category 2
 STOT SE 1: Specific target organ toxicity (single exposure) – Category 1
 Aquatic Chronic 4: Hazardous to the aquatic environment - long-term aquatic hazard – Category 4