

according to Regulation (EC) No. 1907/2006 as amended by (EC) No. 1272/2008

Section 1. Identification of the Substance/Mixture and of the Company/Undertaking

- 1.1 Product Code:** 22144
Product Name: Simeprevir
Synonyms: (2R,3aR,10Z,11aS,12aR,14aR)-N-(cyclopropylsulfonyl)-2,3,3a,4,5,6,7,8,9,11a,12,13,14,14a-tetrahydro-2-[[7-methoxy-8-methyl-2-[4-(1-methylethyl)-2-thiazolyl]-4-quinolinyl]oxy]-5-methyl-4,14-dioxo-cyclopenta[c]cyclopropa[g][1,6]diazacyclotetradecine-12a(1H)-carboxamide; TMC435
- 1.2 Relevant identified uses of the substance or mixture and uses advised against:**
Relevant identified uses: For research use only, not for human or veterinary use.
- 1.3 Details of the Supplier of the Safety Data Sheet:**
Company Name: Cayman Chemical Company
 1180 E. Ellsworth Rd.
 Ann Arbor, MI 48108
Web site address: www.caymanchem.com
Information: Cayman Chemical Company +1 (734)971-3335
- 1.4 Emergency telephone number:**
Emergency Contact: CHEMTREC Within USA and Canada: +1 (800)424-9300
 CHEMTREC Outside USA and Canada: +1 (703)527-3887

Section 2. Hazards Identification

- 2.1 Classification of the Substance or Mixture:**
Skin Corrosion/Irritation, Category 2
Serious Eye Damage/Eye Irritation, Category 1
Respiratory Sensitization, Category 1
Skin Sensitization, Category 1
Germ Cell Mutagenicity, Category 2
Toxic To Reproduction, Category 2
Specific Target Organ Toxicity (single exposure), Category 1
Aquatic Toxicity (Chronic), Category 4
Specific Target Organ Toxicity (single exposure), Category 3
Acute Toxicity: Oral, Category 4

2.2 Label Elements:



GHS Signal Word: **Danger**

GHS Hazard Phrases:

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

GHS Precaution Phrases:

- 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 {hands} thoroughly after handling.
- P270: Do not eat, drink or smoke when using this product.
- P272: Contaminated work clothing should not be allowed out of the workplace.
- P273: Avoid release to the environment.
- P280: Wear {protective gloves/protective clothing/eye protection/face protection}.
- P285: In case of inadequate ventilation wear respiratory protection.

GHS Response Phrases:

- P301+312: IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.
- P302+352: IF ON SKIN: Wash with plenty of soap and water.
- P304+340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
- P305+351+338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- P308+311: If exposed or concerned: Call a {POISON CENTER/Doctor/...}.
- P313: Get medical advice/attention.
- P310: Immediately call a POISON CENTER or doctor/physician.
- P321: Specific treatment {see ... on this label}.
- P330: Rinse mouth.
- P332+313: If skin irritation occurs, get medical advice/attention.
- P333+313: If skin irritation or rash occurs, seek medical advice/attention.
- P342+311: If experiencing respiratory symptoms call a POISON CENTER or doctor/physician.
- P362+364: Take off contaminated clothing and wash it before reuse.

GHS Storage and Disposal Phrases:

- P501: Dispose of contents/container to {...}.

- 2.3 Adverse Human Health** Causes damage to organs.
- Effects and Symptoms:** Causes serious eye damage.
- Causes skin irritation.
- Harmful if swallowed.
- Material may be irritating to the mucous membranes and upper respiratory tract.
- May be harmful by inhalation or skin absorption.
- May cause allergy or asthma symptoms or breathing difficulties if inhaled.
- May cause an allergic skin reaction.
- May cause eye or respiratory system irritation.
- May cause long lasting harmful effects to aquatic life.
- Suspected of causing genetic defects.
- Suspected of damaging fertility or the unborn child.
- To the best of our knowledge, the toxicological properties have not been thoroughly investigated.

Section 3. Composition/Information on Ingredients

CAS # / RTECS #	Hazardous Components (Chemical Name)/ REACH Registration No.	Concentration	EC No./ EC Index No.	GHS Classification
923604-59-5 NA	TMC 435350	100.0 %	NA NA	Skin Corr. 2: H315 Eye Damage 1: H318 Toxic Repro. 2: H361 Resp. Sens. 1: H334 Skin Sens. 1: H317 Mutagen 2: H341

				STOT (SE) 1: H370 Aquatic (C) 4: H413 Acute Tox.(O) 4: H302
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Section 4. First Aid Measures

4.1 Description of First Aid Measures:

In Case of Inhalation: Remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel. Get immediate medical attention.

In Case of Skin Contact: Immediately wash skin with soap and plenty of water for at least 15 minutes. Remove contaminated clothing. Get medical attention if symptoms occur. Wash clothing before reuse.

In Case of Eye Contact: Hold eyelids apart and flush eyes with plenty of water for at least 15 minutes. Have eyes examined and tested by medical personnel.

In Case of Ingestion: Wash out mouth with water provided person is conscious. Never give anything by mouth to an unconscious person. Get medical attention. Do NOT induce vomiting unless directed to do so by medical personnel.

Section 5. Fire Fighting Measures

5.1 Suitable Extinguishing Media: Use alcohol-resistant foam, carbon dioxide, water, or dry chemical spray.
Media: Use water spray to cool fire-exposed containers.
Unsuitable Extinguishing Media: A solid water stream may be inefficient.

5.2 Flammable Properties and Hazards: No data available.
Hazards: No data available.
Flash Pt: No data.
Explosive Limits: LEL: No data. UEL: No data.
Autoignition Pt: No data.

5.3 Fire Fighting Instructions: As in any fire, wear self-contained breathing apparatus pressure-demand (NIOSH approved or equivalent), and full protective gear to prevent contact with skin and eyes.

Section 6. Accidental Release Measures

6.1 Protective Precautions, Protective Equipment and Emergency Procedures: Avoid raising and breathing dust, and provide adequate ventilation. As conditions warrant, wear a NIOSH approved self-contained breathing apparatus, or respirator, and appropriate personal protection (rubber boots, safety goggles, and heavy rubber gloves).

6.2 Environmental Precautions: Take steps to avoid release into the environment, if safe to do so.

6.3 Methods and Material For Containment and Cleaning Up: Contain spill and collect, as appropriate. Transfer to a chemical waste container for disposal in accordance with local regulations.

Section 7. Handling and Storage

7.1 Precautions To Be Taken in Handling: Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid prolonged or repeated exposure.

7.2 Precautions To Be Taken in Storing: Keep container tightly closed. Store in accordance with information listed on the product insert.

Section 8. Exposure Controls/Personal Protection

8.1 Exposure Parameters:

8.2 Exposure Controls:

8.2.1 Engineering Controls (Ventilation etc.): Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits.

8.2.2 Personal protection equipment:

Eye Protection: Safety glasses

Protective Gloves: Compatible chemical-resistant gloves

Other Protective Clothing: Lab coat

Respiratory Equipment (Specify Type): NIOSH approved respirator, as conditions warrant.

Work/Hygienic/Maintenance Practices: Do not take internally.

Facilities storing or utilizing this material should be equipped with an eyewash and a safety shower.
Wash thoroughly after handling.

No data available.

Section 9. Physical and Chemical Properties

9.1 Information on Basic Physical and Chemical Properties

Physical States: [] Gas [] Liquid [X] Solid

Appearance and Odor: A solid

pH: No data.

Melting Point: No data.

Boiling Point: No data.

Flash Pt: No data.

Evaporation Rate: No data.

Flammability (solid, gas): No data available.

Explosive Limits: LEL: No data. UEL: No data.

Vapor Pressure (vs. Air or mm Hg): No data.

Vapor Density (vs. Air = 1): No data.

Specific Gravity (Water = 1): No data.

Solubility in Water: No data.

Solubility Notes: Soluble in: DMSO; chloroform; ethyl acetate;

Octanol/Water Partition Coefficient: No data.

Autoignition Pt: No data.

Decomposition Temperature: No data.

Viscosity: No data.

9.2 Other Information

Percent Volatile: No data.

Molecular Formula & Weight: C38H47N5O7S2 749.9

Section 10. Stability and Reactivity

- 10.1 Reactivity:** No data available.
- 10.2 Stability:** Unstable [] Stable [X]
- 10.3 Stability Note(s):** Stable if stored in accordance with information listed on the product insert.
- Polymerization:** Will occur [] Will not occur [X]
- 10.4 Conditions To Avoid:** No data available.
- 10.5 Incompatibility - Materials To Avoid:** strong oxidizing agents
- 10.6 Hazardous Decomposition or Byproducts:** carbon dioxide
carbon monoxide
hydrogen sulfide
nitrogen oxides

Section 11. Toxicological Information

- 11.1 Information on Toxicological Effects:** The toxicological effects of this product have not been thoroughly studied.

CAS #	Hazardous Components (Chemical Name)	NTP	IARC	ACGIH	OSHA
923604-59-5	TMC 435350	n.a.	n.a.	n.a.	n.a.

Section 12. Ecological Information

- 12.1 Toxicity:** Avoid release into the environment.
Runoff from fire control or dilution water may cause pollution.
- 12.2 Persistence and Degradability:** No data available.
- 12.3 Bioaccumulative Potential:** No data available.
- 12.4 Mobility in Soil:** No data available.
- 12.5 Results of PBT and vPvB assessment:** No data available.
- 12.6 Other adverse effects:** No data available.

Section 13. Disposal Considerations

- 13.1 Waste Disposal Method:** Dispose in accordance with local, state, and federal regulations.

Section 14. Transport Information

- 14.1 LAND TRANSPORT (US DOT):**
- DOT Proper Shipping Name:** Not dangerous goods.
- DOT Hazard Class:**
- UN/NA Number:**
- 14.1 LAND TRANSPORT (European ADR/RID):**
- ADR/RID Shipping Name:** Not dangerous goods.
- UN Number:**
- Hazard Class:**

14.3 AIR TRANSPORT (ICAO/IATA):

ICAO/IATA Shipping Name: Not dangerous goods.

Additional Transport Information: Transport in accordance with local, state, and federal regulations.

Section 15. Regulatory Information

EPA SARA (Superfund Amendments and Reauthorization Act of 1986) Lists

CAS #	Hazardous Components (Chemical Name)	S. 302 (EHS)	S. 304 RQ	S. 313 (TRI)
923604-59-5	TMC 435350	No	No	No

CAS #	Hazardous Components (Chemical Name)	Other US EPA or State Lists
923604-59-5	TMC 435350	CAA HAP,ODC: No; CWA NPDES: No; TSCA: No; CA PROP.65: No

Regulatory Information Statement: This SDS was prepared in accordance with 29 CFR 1910.1200 and Regulation (EC) No.1272/2008.

Section 16. Other Information

Revision Date: 08/23/2017

Additional Information About This Product: No data available.

Company Policy or Disclaimer: DISCLAIMER: This information is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes.