



Safety Data Sheet - Version 5.0

Preparation Date 5/15/2015

Latest Revision Date (If Revised)

SDS Expiry Date 5/13/2018

1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1 Product Identifier

Chemical Name Simeprevir

Catalogue # S466500

1.2 Relevant Identified Uses of the Substance or Mixture and Uses Advised Against

Product Uses To be used only for scientific research and development. Not for use in humans or animals.

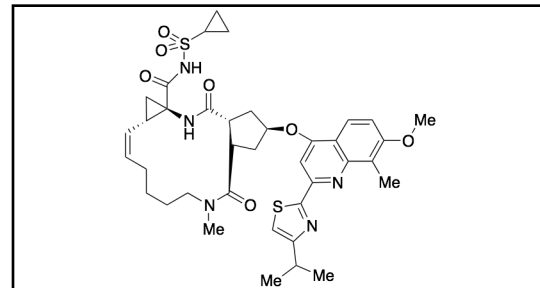
1.3 Details of the Supplier of the Safety Data Sheet

Company Toronto Research Chemicals
2 Brisbane Road
Toronto, ON M3J 2J8
CANADA

Telephone +14166659696

FAX +14166654439

Email orders@trc-canada.com



1.4 Emergency Telephone Number

Emergency# +14166659696 between 0800-1700 (GMT-5)

2. HAZARDS IDENTIFICATION

WHMIS Classification (Canada)

D1B Toxic Material Causing Immediate and Serious Toxic Effects
Toxic by Ingestion

WHMIS Symbols (Canada)



2.1/2.2 Classification of the Substance or Mixture and Label Elements

GHS Hazards Classification (According to EU Regulation 1272/2008 and US OSHA 1910.1200)

Acute Toxicity, Oral (Category 4)

Hazardous to the Aquatic Environment, Acute Hazard (Category 1)

Hazardous to the Aquatic Environment, Long-Term Hazard (Category 1)

EU Classification (According to EU Regulation 67/548/EEC)

Harmful if swallowed. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

EU Risk and Safety Statements (According to EU Regulation 67/548/EEC)

Hazard Statements Hazard Codes

Harmful

Xn



Environmental Hazard

N



Risk Codes and Phrases

R22

Harmful if swallowed.

R50/53

Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Safety Precaution Codes and Phrases

S46

If swallowed, seek medical advice immediately and show this container or label.

S61

Avoid release to the environment. Refer to special instructions.

GHS Hazards Identification (According to EU Regulation 1272/2008 and US OSHA 1910.1200)

Signal Word Warning



GHS Hazard Statements

H302 Harmful if swallowed.
H400 Very toxic to aquatic life.
H410 Very toxic to aquatic life with long lasting effects.

GHS Precautionary Statements

P264 Wash hands thoroughly after handling.
P273 Avoid release to the environment.
P301/P312 IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.
P391 Collect spillage.

2.3 Unclassified Hazards/Hazards Not Otherwise Classified

No data available

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Molecular Formula: C₃₈H₄₇N₅O₇S₂

Molecular Weight: 749.94

CAS Registry #: 923604-59-5

EC#:

Synonyms

(2R,3aR,10Z,11aS,12aR,14aR)-N-(Cyclopropylsulfonyl)-2,3,3a,4,5,6,7,8,9,11a,12,13,14,14a-tetradecahydro-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; TMC 435; TMC 435350;

3.2 Mixtures

Not a mixture

4. FIRST AID MEASURES

4.1 Description of First Aid Measures

General Advice

If medical attention is required, show this safety data sheet to the doctor.

If Inhaled

If inhaled, move casualty to fresh air. If not breathing, give artificial respiration and consult a physician.

In Case of Skin Contact

Wash affected area with soap and water. Consult a physician if any exposure symptoms are observed.

In Case of Eye Contact

Immediately rinse eyes with plenty of water for at least 15 minutes. Consult a physician.

If Swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Do NOT induce vomiting unless advised to do so by a physician or Poison Control Center. Seek medical attention.

4.2 Most Important Symptoms and Effects, Both Acute and Delayed

No data available

4.3 Indication of any Immediate Medical Attention and Special Treatment Needed

No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing Media

Suitable Extinguishing Media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special Hazards Arising from the Substance or Mixture

Carbon oxides, Nitrogen oxides, Sulfur oxides

5.3 Advice for Firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further Information

No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal Precautions, Protective Equipment and Emergency Procedures

Use recommended personal protective equipment (see Section 8). Prevent the formation of dusts and mists. Adequate ventilation must be provided to ensure dusts or mists are not inhaled.

6.2 Environmental Precautions

Material should not be allowed to enter the environment. Prevent further spillage or discharge into drains, if safe to do so.

6.3 Methods and Materials for Containment and Cleaning Up

Contain the spill and then collect using non-combustible absorbent material (such as clay, diatomaceous earth, vermiculite or other appropriate material). Place material in a suitable, sealable container and then dispose according to local/national regulations and guidance (see Section 13).

For protective equipment, refer to Section 8. For disposal, see Section 13.

7. HANDLING AND STORAGE

7.1 Precautions for Safe Handling

Avoid contact with skin and eyes. Ventilation and proper handling are to be used to prevent the formation of dusts and mists. Normal measures for preventative fire protection. No smoking, eating or drinking around this material. Wash hands after use.

7.2 Conditions for Safe Storage, Including any Incompatibilities

Ensure container is kept securely closed before and after use. Keep in a well ventilated area and do not store with strong oxidizers or other incompatible materials (see Section 10).

Storage conditions: Refrigerator

7.3 Specific End Uses

For scientific research and development only. Not for use in humans or animals.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control Parameters

Contains no components with established occupation exposure limits.

8.2 Exposure Controls

Appropriate Engineering Controls

A laboratory fumehood or other appropriate form of local exhaust ventilation should be used to avoid exposure.

Personal Protective Equipment

All recommendations below are advisory in nature and a risk assessment should be performed by the employer/end user prior to use of this product. The type of protective equipment must be selected based on the amount and concentration of the dangerous material being used in the workplace.

Eye/Face Protection

Safety glasses or safety goggles. All equipment should have been tested and approved under appropriate standards, such as NIOSH (US), CSA (Canada), or EN 166 (EU).

Skin Protection

Gloves should be used when handling this material. Gloves are to be inspected prior to use. Contaminated gloves are to be removed using proper glove removal technique so that the outer surface of the glove does not contact bare skin. Dispose of contaminated gloves after use in compliance with good laboratory practices and local requirements.

Gloves used for incidental exposures (splash protection) should be designated as "low chemical resistant" or "waterproof" by EU standard EN 374. Unrated gloves are not recommended.

Suggested gloves: AnsellPro nitrile gloves style 92-500 or 92-600, 5 mil thickness.

Penetration time has not been determined.

Gloves used for prolonged direct exposure (immersion) should be designated "chemical resistant" as per EN 734 with the resistance codes corresponding to the anticipated use of the material.

Suggested gloves: AnsellPro Viton/Butyl gloves style 38-612, 4/8 mil thickness.

Penetration time has not been determined.

These recommendations may not apply if the material is mixed with any other chemical, or dissolved into a solution. A risk assessment must be performed to ensure the gloves will still offer acceptable protection.

Body Protection

Fire resistant (Nomex) lab coat or coveralls.

Respiratory Protection

Recommended respirators are NIOSH-approved N95 or CEN-approved FFP2 particulate respirators. These are to be only used as a backup to local exhaust ventilation or other engineering controls. If the respirator is the only means of protection, a full-face supplied air respirator must be used.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on Basic Physical and Chemical Properties

A) Appearance

Off White Solid

C) Odour Threshold

No data available

E) Melting Point/Freezing Point

>225°C (dec.)

G) Flash point

No data available

I) Flammability (Solid/Gas)

No data available

K) Vapour Pressure

No data available

M) Relative Density

No data available

O) Partition Coefficient: n-octanol/water

No data available

Q) Decomposition Temperature

No data available

S) Explosive Properties

No data available

B) Odour

No data available

D) pH

No data available

F) Initial Boiling Point/Boiling Range

No data available

H) Evaporation Rate

No data available

J) Upper/Lower Flammability/Explosive Limits

No data available

L) Vapour Density

No data available

N) Solubility

Chloroform, DMSO, Ethyl Acetate

P) Auto-Ignition Temperature

No data available

R) Viscosity

No data available

T) Oxidizing Properties

No data available

9.2 Other Information

no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical Stability

Stable at recommended storage conditions.

10.3 Possibility of Hazardous Reactions

No data available

10.4 Conditions to Avoid

No data available

10.5 Incompatible Materials

Strong oxidizing materials.

10.6 Hazardous Decomposition Products

No data available

11. TOXICOLOGICAL INFORMATION

11.1 Information on Toxicological Effects

A) Acute Toxicity

No data available

B) Skin Corrosion/Irritation

No data available

C) Serious Eye Damage/Irritation

No data available

D) Respiratory or Skin Sensitization

No data available

E) Germ Cell Mutagenicity

No data available

F) Carcinogenicity

No data available

G) Reproductive Toxicity/Teratogenicity

No data available

H) Single Target Organ Toxicity - Single Exposure

No data available

I) Single Target Organ Toxicity - Repeated Exposure

No data available

J) Aspiration Hazard

No data available

K) Potential Health Effects and Routes of Exposure

Inhalation

May be harmful if inhaled. May cause respiratory tract irritation.

Ingestion

Harmful if swallowed.

Skin

May be harmful if absorbed through skin. May cause skin irritation.

Eyes

May cause eye irritation.

L) Signs and Symptoms of Exposure

No data available

To the best of our knowledge, the chemical, physical, and toxicological properties of this material have not been thoroughly investigated.

M) Additional Information

RTECS: Not listed

12. ECOLOGICAL INFORMATION

12.1 Toxicity

No data available

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

13. DISPOSAL CONSIDERATIONS

13.1 Waste Treatment Methods

A) Product

Product may be burned in an incinerator equipped with afterburner and scrubber. Excess and expired materials are to be offered to a licensed hazardous material disposal company. Ensure that all Federal and Local regulations regarding the disposal and destruction of this material are followed.

B) Contaminated Packaging

Dispose of as above.

C) Other Considerations

Product is not to be disposed of in sanitary sewers, storm sewers, or landfills.

14. TRANSPORT INFORMATION**14.1 UN Number**

DOT (US): 3077 IATA: 3077 IMDG: 3077 ADR/RID: 3077

14.2 UN Proper Shipping Name

DOT (US)/IATA:

Environmentally hazardous substance, solid, n.o.s. (Simeprevir)

IMDG/ARD/RID:

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Simeprevir)

14.3 Transport Hazard Class(es)

DOT (US): N/A IATA: 9 IMDG: 9 ADR/RID: 9

14.4 Packing Group

DOT (US): N/A IATA: III IMDG: III ADR/RID: III

14.5 Environmental Hazards

DOT (US): None IATA: None IMDG: None ADR/RID: None

14.6 Special Precautions for User

None

15. REGULATORY INFORMATION

This safety data sheet complies with the requirements of WHMIS (Canada), OSHA 1910.1200 (US), and EU Regulation EC No. 1907/2006 (European Union).

15.1 Safety, Health and Environmental Regulations/Legislation Specific for the Substance or Mixture**A) Canada**

DSL/NDSL Status: This product is not listed on the Canadian DSL/NDSL.

B) United States

TSCA Status: This product is not listed on the US EPA TSCA.

C) European Union

ECHA Status: This product is not registered with the EU ECHA.

15.2 Chemical Safety Assessment

No data available

16. OTHER INFORMATION**16.1 Revision History**

Original Publication Date: 5/15/2015

16.2 List of Abbreviations

LD50	Median lethal dose of a substance required to kill 50% of a test population.
LC50	Medial lethal concentration of a substance required to kill 50% of a test population.
LDLo	Lowest known lethal dose
TDLo	Lowest known toxic dose
IARC	International Agency for Research on Cancer
NTP	National Toxicology Program
RTECS	Registry of Toxic Effects of Chemical Substances

16.3 Further Information

Copyright 2015. Toronto Research Chemicals Inc. Copies may be made for internal use only. The above information is believed to be correct to the best of our knowledge, but is to be only used as a guide. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Please take all due care when handling this product.