



Material Safety Data Sheet (MSDS)

Version 2.1 Revision Date: 04/21/2017

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifier

Product Name: Simurosertib

Catalog No.: V4595

CAS No.: 1330782-76-7

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses: Laboratory chemicals, synthesis of substances.

1.3 Details of the supplier of the safety data sheet

Company: InvivoChem LLC

Tel: +1 708 310-1919

Fax: +1 708 557-7486

1.4 Emergency telephone number

Emergency phone #: +1 708 310-1919

2. COMPOSITION/INFORMATION ON INGREDIENTS

2.1 Substances

Formula: C₁₇H₁₉N₅O₅

Molecular Weight: 341.433

3. PHYSICAL AND CHEMICAL PROPERTIES

3.1 Information on basic physical and chemical properties

(a) Appearance	Solid
(b) Odor	No data available
(c) Odor threshold	No data available
(d) pH	No data available
(e) Melting/freezing point	No data available
(f) Boiling point/range	No data available
(g) Flash point	No data available
(h) Evaporation rate	No data available
(i) Flammability (solid, gas)	No data available
(j) Upper/lower flammability or explosive limits	No data available
(k) Vapor pressure	No data available
(l) Vapor density	No data available
(m) Relative density	No data available
(n) Water solubility	N/A
(o) Partition coefficient	No data available
(p) Auto-ignition temperature	No data available
(q) Decomposition temperature	No data available
(r) Viscosity	No data available

(s) **Explosive properties** No data available

(t) **Oxidizing properties** No data available

3.2 Other Safety Information

No data available

4. HAZARDS IDENTIFICATION

4.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

4.2 GHS Label elements, including precautionary statements

Pictogram



Signal word Danger

Hazard statement(s)

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.

Precautionary statement(s)

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 skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/ eye protection/ face protection.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position 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.
P312 Call a POISON CENTER or doctor/ physician if you feel unwell.
P321 Specific treatment (see supplemental first aid instructions on this label).
P332 + P313 If skin irritation occurs: Get medical advice/ attention.
P337 + P313 If eye irritation persists: Get medical advice/ attention.
P362 Take off contaminated clothing and wash before reuse.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

P405

Store locked up.

P501

Dispose of contents/ container to an approved waste disposal plant.

4.3 Other hazards

None.

5. FIRST AID MEASURES

5.1 Description of first aid measures

In case of eye contact

Remove any contact lenses, locate eye-wash station, and flush eyes immediately with large amounts of water for 15 minutes. Separate eyelids with fingers to ensure adequate flushing. Promptly consult a physician.

In case of skin contact

Wash off thoroughly with soap and large amounts of water. Remove contaminated clothing and shoes and call a physician.

If inhaled

Immediately relocate victim to fresh air. If breathing is difficult, give cardiopulmonary resuscitation (CPR). Avoid mouth-to-mouth resuscitation.

If swallowed

Wash out mouth with water; Do NOT induce vomiting; call a physician promptly.

5.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labeling (see section 4.2).

5.3 Indication of any immediate medical attention and special treatment needed

No data available.

6. FIRE FIGHTING MEASURES

6.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical, foam, and carbon dioxide fire extinguisher.

6.2 Special hazards arising from the substance or mixture

No data available.

6.3 Advice for firefighters

Wear self-contained breathing apparatus and protective clothing if necessary.

7. ACCIDENTAL RELEASE MEASURES

7.1 Personal precautions, protective equipment and emergency procedures

Use full personal protective equipment. Avoid dust formation, avoid breathing vapors, mist, dust or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

Refer to protective measures listed in sections 9.

7.2 Environmental precautions

Try to prevent further leakage or spillage if safe to do so. Keep the product away from drains or water courses.

7.3 Methods and materials for containment and cleaning up

Absorb solutions with finely-powdered liquid-binding material (diatomite, universal binders); Decontaminate surfaces and equipment by scrubbing with alcohol; Pick up and arrange disposal without creating dust; Keep in suitable, closed containers for disposal; Dispose of contaminated material according to Section 13.

8. HANDLING AND STORAGE

8.1 Precautions for safe handling

Avoid inhalation, contact with eyes and skin. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. Use only in areas with appropriate exhaust ventilation.

8.2 Conditions for safe storage, including any incompatibilities

Keep container tightly sealed in cool, dry, and well-ventilated area. Keep away from direct sunlight and

sources of ignition.

Recommended storage temperature: 2 - 8 °C for short term (weeks to 3 months) or -20°C for long term (3 months to years).

8.3 Specific end use(s)

No data available.

9. EXPOSURE CONTROLS/PERSONAL PROTECTION

9.1 Control parameters

Components with workplace control parameters

This product contains no substances with occupational exposure limit values.

9.2 Exposure controls

Engineering controls

Ensure adequate ventilation. Provide accessible safety shower and eye wash station. Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection	Face shield and safety goggles with side-shields.
Hand protection	Protective gloves.
Skin and body protection	Impervious clothing.
Respiratory protection	Suitable respirator.
Environmental exposure controls	Keep the product away from drains, water courses or the soil. Clean spillages in a safe way as soon as possible.

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available.

10.2 Chemical stability

Stable under 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 acids/alkalis, strong oxidizing/reducing agents.

10.6 Hazardous decomposition products

Under fire conditions, may decompose and emit toxic fumes.

Other decomposition products - no data available.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Classified based on available data. For more details, see section 4.

Skin corrosion/irritation

Classified based on available data. For more details, see section 4.

Serious eye damage/irritation

Classified based on available data. For more details, see section 4.

Respiratory or skin sensitization

Classified based on available data. For more details, see section 4.

Germ cell mutagenicity

Classified based on available data. For more details, see section 4.

Carcinogenicity

IARC: No component of this product present at a level equal to or greater than 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at a level equal to or greater than 0.1% is identified as a potential or confirmed carcinogen by ACGIH.

NTP: No component of this product present at a level equal to or greater than 0.1% is identified as a anticipated or confirmed carcinogen by NTP.

OSHA: No component of this product present at a level equal to or greater than 0.1% is identified as a potential or confirmed carcinogen by OSHA.

Reproductive toxicity

Classified based on available data. For more details, see section 4.

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 4.

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 4.

Aspiration hazard

Classified based on available data. For more details, see section 4.

Additional information

RTECS No.: Unavailable

This information is based on our current knowledge. However the chemical, physical, and toxicological properties have not been completely investigated.

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

PBT/vPvB assessment not available as chemical safety assessment not required or not conducted.

12.6 Other adverse effects

No data available.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Dispose substance in accordance with prevailing country, federal, state and local regulations. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Conduct recycling or disposal in accordance with prevailing country, federal, state and local regulations.

14. TRANSPORT INFORMATION DOT

(US)

This substance is considered to be non-hazardous/not dangerous for transport.

IMDG

This substance is considered to be non-hazardous/not dangerous for transport.

IATA

This substance is considered to be non-hazardous/not dangerous for transport.

15. REGULATORY INFORMATION

SARA 302 Components:

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components:

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards:

Acute Health Hazard, Chronic Health Hazard.

Massachusetts Right To Know Components:

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components:

No components are subject to the Pennsylvania Right to Know Act.

New Jersey Right To Know Components:

No components are subject to the New Jersey Right to Know Act.

California Prop. 65 Components:

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. The product is for research use only and for trained personnel. The burden of safe use of this material rests entirely with the user. InvivoChem LLC shall not be held liable for any damage resulting from handling or from contact with the above product.