

SAFETY DATA SHEET (SDS)

RepSox

1. Identification

Product Name: RepSox

Product Code: TB47964

CAS No.: 446859-33-2

Molecular Formula: C₁₇H₁₃N₅

Molecular Weight: 287.32

Product Use: For Research Use Only (RUO). Laboratory chemical; manufacture of substances.

Uses Advised Against: Any use other than the identified research use.

Distributed by: Trailhead Biosystems Inc.

23215 Commerce Park Road, Beachwood, Ohio, 44122

SDSs are available at the following website: www.trailbio.com

Company Phone Number: +1 (216) 490-3304

Emergency Telephone Number: +1-800-424-9300

Email: support@trailbio.com

2. Hazard(s) Identification

Classification (OSHA HCS 2024, GHS Rev. 7; 29 CFR 1910.1200)

Acute toxicity, oral – Category 3, H301

Hazards not otherwise classified (HNOC)

None.

GHS Label Elements

Pictogram:



Signal Word: Danger

Hazard Statements

H301 – Toxic if swallowed

Precautionary Statements – Prevention

P264 – Wash hands thoroughly after handling.

P270 – Do not eat, drink or smoke when using this product.

Precautionary Statements – Response

P330 – Rinse mouth.

Precautionary Statements – Storage

P405 – Store locked up.

Precautionary Statements – Disposal

P501 – Dispose of contents/container in accordance with local regulations.

3. Composition/Information on Ingredients

Substance

Chemical Name: E-616452

CAS No.: 446859-33-2

Molecular Formula: C₁₇H₁₃N₅

Molecular Weight: 287.32

Single substance supplied at ≥ 98% (as supplied). See Section 2 for hazard classification.

4. First-Aid Measures

Description of first-aid measures**Eye Contact**

Where Diphoterine is not available, locate eye-wash station, rinse eyes with copious amounts of water for at least 20 minutes. Promptly call a physician.

Skin Contact

Where Diphoterine is not available, rinse skin with copious amounts of water for at least 20 minutes. Remove contaminated clothing and shoes and call a physician.

Inhalation

Immediately relocate self or casualty to fresh air and keep comfortable for breathing. If experiencing respiratory problems, promptly call a physician.

Ingestion

Where Diphoterine is not available, rinse mouth with copious amounts of water. Seek urgent medical advice.

Most important symptoms/effects, acute and delayed

The most important known symptoms and effects are described in the labelling (see Section 2). See Section 2 for hazard classification.

Indication of immediate medical attention and special treatment needed

No special immediate treatment required

5. Fire-Fighting Measures

Suitable Extinguishing Media

Carbon dioxide (CO₂), alcohol-resistant foam, dry chemical powder, or water spray.

Unsuitable Extinguishing Media

None known.

Specific hazards arising from the chemical

Thermal decomposition can lead to release of irritating gases and vapors.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Remove undamaged containers from fire area if safe to do so.

6. Accidental Release Measures

Personal precautions, protective equipment, and emergency procedures

Use full personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist, or gas. Ensure adequate ventilation. Keep personnel away from spill/leak. Refer to protective measures listed in Section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Prevent product from entering drains, waterways, or sewer systems. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Methods for Containment

Prevent further leakage or spillage if safe to do so.
Remove all sources of ignition.

Methods for Cleaning Up

Absorb spilled material with an inert absorbent (e.g. sand, silica gel, vermiculite) before transferring into an airtight container. Dispose of appropriately according to local regulations.

7. Handling and Storage

Precautions for safe handling

Wear appropriate personal protective equipment. Use only under a chemical fume hood. Keep away from heat/sparks/open flame/hot surfaces. Take measures to prevent the build-up of electrostatic charge. Ensure adequate exhaust ventilation, especially if dust, aerosol or fumes will be generated. Avoid contact with skin, eyes and clothing. For precautions see section 2.

Conditions for safe storage, including any incompatibilities

Keep container tightly sealed in a cool, well-ventilated area. Keep away from direct sunlight and sources of ignition.

Recommended storage temperature (powder): –20 °C – 3 years; 4 °C – 2 years

Recommended storage temperature (in solvent): –80 °C – 2 years; –20 °C – 1 year

Shipping: Ambient temperature if less than 2 weeks.

8. Exposure Controls/Personal Protection

Control parameters

Exposure Guidelines

This product contains no substances with established occupational exposure limit (OEL) values.

Appropriate engineering controls

Use only under a chemical fume hood ensuring adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting/equipment. Ensure that eyewash stations and safety showers are close to the workstation.

Individual protection measures, such as personal protective equipment

Eye/face protection

Safety goggles with side-shields.

Hand protection

Protective (impervious) gloves.

Skin and body protection

Impervious clothing.

Respiratory protection

Suitable respirator where dust, aerosol or fume may be generated.

General Hygiene Considerations

Handle in accordance with good industrial hygiene and safety practice. Wash hands before and after use. Do not eat, drink or smoke when using this product. Ensure hair or skin particles cannot enter the chemical container.

Environmental exposure controls

Avoid discharge into the environment. Keep product away from drains, water courses, and soil. Clean spillages safely as soon as possible.

9. Physical and Chemical Properties

Appearance: Solid

Odor: No data available

Odor Threshold: No data available

pH: No data available

Melting point/freezing point: 195°C

Boiling point/boiling range: 501.9±50.0°C at 760 mmHg

Flash Point: No data available

Evaporation Rate: No data available

Flammability (solid, gas): No data available

Upper/lower flammability or explosive limits: No data available

Vapor Pressure: No data available

Vapor Density: No data available

Relative Density: No data available

Solubility: No data available

Partition Coefficient (n-octanol/water): No data available

Autoignition temperature: No data available

Decomposition temperature: No data available

Viscosity: No data available

Explosive properties: No data available

Oxidizing properties: No data available

Molecular Weight: 287.32

10. Stability and Reactivity

Reactivity

No data available.

Chemical Stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

None under normal storage conditions.

Conditions to avoid

Heat, sparks, open flames, sources of ignition. Exposure to moisture

Incompatible Materials

Strong acids/alkalis, strong oxidizing/reducing agents.

Hazardous Decomposition Products

Under fire conditions, may decompose and emit toxic fumes.

11. Toxicological Information

Information on toxicological effects

Acute toxicity (oral)

Classified as Category 3 (H301); see Section 2.

Skin corrosion/irritation

No toxicological data available for this product.

Serious eye damage/irritation

No toxicological data available for this product.

Respiratory or skin sensitization

Toxic if swallowed.

Germ cell mutagenicity

No toxicological data available for this product.

Reproductive Toxicity

No toxicological data available for this product.

STOT – single exposure

No toxicological data available for this product.

STOT – repeated exposure

No toxicological data available for this product.

Aspiration hazard

No toxicological data available for this product.

Carcinogenicity

No toxicological data available for this product.

Additional information

RTECS No.: Not available. This information is based on current knowledge; the chemical, physical, and toxicological properties have not been completely investigated.

12. Ecological Information

Ecotoxicity

No data available.

Persistence and degradability

No Ecological data available for this product.

Bioaccumulative potential

No Ecological data available for this product.

Mobility in soil

No Ecological data available for this product.

Results of PBT and vPvB assessment

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

Other adverse effects

No data available.

13. Disposal Considerations

Waste treatment methods

Ensure product is disposed of by licensed waste carriers in accordance with prevailing country, federal, state, and local regulations.

Contaminated packaging

Ensure inner packaging is disposed of by licensed waste carriers. Some outer packaging may be recyclable if not contaminated.

14. Transport Information

DOT:

Proper shipping name: Toxic substances

UN number: 2811

Class: 6.1

Packing group: III

TDG: Not determined

MEX: Not determined

ICAO: Not determined

IATA:

Proper shipping name: Toxic substances

UN number: 2811

Class: 6.1

Packing group: III

IMDG:

Proper shipping name: Toxic substances

UN number: 2811

Class: 6.1

Packing group: III

ADR/RID: Not determined

ADN: Not determined

15. Regulatory Information

U.S. Federal Regulations

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

SARA 313: This material does not contain any chemical components with known CAS numbers above De Minimis reporting levels under SARA Title III, Section 313.

SARA 311/312 Hazards: No SARA Hazards.

US State Regulations

California Proposition 65: This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or other reproductive harm.

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

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

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

16. Other Information

Prepared By	Trailhead Biosystems
Preparation Date	2026-09-02
Revision Date	2026-09-02
Revision Note	No information available

Disclaimer: The information provided in this Safety Data Sheet (SDS) is correct to the best of our knowledge. The information given is designed only as guidance for safe handling, use, processing, storage, transportation, disposal, and release and is not to be considered a warranty or quality specification. This product is For Research Use Only and must be handled only by suitably qualified, experienced personnel in appropriately equipped facilities. The burden of safe use of this material rests with the user. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text.

END