



SAFETY DATA SHEET

Generic SDS (EU) - No country specific data

Version 5.8. Revision Date 2021.03.10

Issued on 2025.02.07

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product Name: 2-{1-benzyl-3-methyl-2,4,6-trioxo-1H,2H,3H,4H,5H,6H,7H-pyrrolo[2,3-d]pyrimidin-5-yl}acetic acid

Product Catalogue Number: EN300-04693

EC number: N/A

REACH No.: A registration number for this substance / mixture is not available. The substance is exempted from registration as the annual tonnage does not require a registration or registration is envisaged for a later registration deadline.

Alias product code(s): N/A

1.2 Recommended use of the substance and restrictions on use

Recommended use: Laboratory chemicals, research and development use only.

1.3 Supplier's details

Company: ENAMINE Ltd. 78 Winston Churchill Street 02094 Kyiv Ukraine

Telephone: +380 44 5373218

Fax: +380 44 5373253

E-mail address: SDS@enamine.net

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance / mixture

Classification according to Regulation (EC) No 1272/2008

Acute toxicity, oral (Category 4), H302

Acute toxicity, dermal (Category 4), H312

Acute toxicity, inhalation (Category 4), H332

For the full text of the H-Statements mentioned in this Section, see Section 2.2.

2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008

Pictogram:



Signal word: Warning

Hazard statement(s):

H302 Harmful if swallowed
H312 Harmful in contact with skin
H332 Harmful if inhaled

Precautionary statements:

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P264 Wash hands thoroughly after handling. Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P301+P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell.
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.
P330 Rinse mouth.
P363 Wash contaminated clothing before reuse.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

2.3 Other hazards

N/A

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

| | |
|-------------------|---|
| Synonyms: | N/A |
| Formula: | C ₁₆ H ₁₅ N ₃ O ₅ |
| Molecular Weight: | 329.3081 |

Hazardous ingredients according to Regulation (EC) No 1272/2008

Component: 2-{1-benzyl-3-methyl-2,4,6-trioxo-1H,2H,3H,4H,5H,6H,7H-pyrrolo[2,3-d]pyrimidin-5-yl}acetic acid

Classification:

Acute toxicity, oral (Category 4), H302

Acute toxicity, dermal (Category 4), H312
Acute toxicity, inhalation (Category 4), H332

4. FIRST AID MEASURES

4.1 Description of first aid measures

| | |
|-----------------|---|
| General advice: | Consult a physician. Show this safety data sheet to the doctor in attendance. |
| Inhalation: | If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen. Seek medical attention immediately. |
| Skin contact: | In case of skin contact, flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Call a physician. |
| Eye contact: | In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician. |
| Ingestion: | If swallowed, wash out mouth with water provided person is conscious. Call a physician. |

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labeling (see section 2.2) and/or in section 11.

4.3 Indication of any immediate medical attention and special treatment needed

No data available

5. FIREFIGHTING MEASURES

5.1 Suitable extinguishing media

Sand, carbon dioxide, dry chemical powder, or appropriate foam.

5.2 Specific hazards arising from the substance or mixture

May emit toxic fumes under fire conditions including .

5.3 Special protective equipment and precautions for firefighters

Fire-extinguishing work is done from the windward and the suitable fire-extinguishing method according to the surrounding situation is used. Uninvolved persons should evacuate to a safe place. In case of fire in the surroundings: remove movable containers if safe to do so.

Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Wipe dry, place a rag in a bag and hold for waste disposal. Avoid fumes inhaling. Ventilate area and wash spill site after material pickup is complete.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Handling is performed in a well ventilated place. Wear suitable protective equipment. Do not breathe vapor. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure. Wash hands and face thoroughly after handling.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed and upright. Avoid overheating. Store in a dry and well-ventilated place at .

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

N/A

8.2 Appropriate engineering controls

Install a closed system or local exhaust so that workers should not be exposed directly.

Install safety shower and eye bath.

Wash hands thoroughly after handling.

8.3 Personal protective equipment

Respiratory Protection: Government approved respirator.

Skin Protection: Compatible chemical-resistant gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Wash and dry hands.

Eye/Face Protection: Government approved eye/face protection equipment.

Body protection: Protective clothing. Protective boots, if the situation requires.

9. PHYSICAL AND CHEMICAL PROPERTIES

Property Value At Temperature or Pressure

Appearance (20°C)

Physical state: N/A

Odour: N/A

Colour: N/A

pH: N/A

Melting point/freezing point (°C): N/A

Initial boiling point and boiling point range (°C):

Flash Point (°C): N/A

Vapour pressure: N/A

Vapour density: N/A

Relative density (g/ml): N/A

Partition coefficient: n-octanol/water: 0.411

| | |
|---------------------------------|-----|
| Auto-ignition temperature (°C): | N/A |
| Viscosity: | N/A |
| Flammability: | N/A |
| Explosive properties: | N/A |
| Oxidizing properties: | N/A |
| Water solubility: | N/A |
| Evaporation rate: | N/A |
| Refractive index: | |

10. STABILITY AND REACTIVITY

10.1 Chemical stability

Stable under specified storage temperature.

10.2 Possibility of hazardous reactions

No data available

10.3 Conditions to avoid

No data available

10.4 Incompatible materials

Strong oxidizing agents.

10.5 Hazardous decomposition products

11. TOXICOLOGICAL INFORMATION

N/A

12. ECOLOGICAL INFORMATION

N/A

13. DISPOSAL CONSIDERATIONS

| | |
|----------------------------------|---|
| Substance disposal: | 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. Observe all federal, state, and local environmental regulations |
| Contaminated packaging disposal: | Dispose of as unused product |

14. TRANSPORT INFORMATION

14.1 UN number

ADR/RID: -

IMDG: -

IATA: -

14.2 UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

14.3 Transport hazard class(es)

ADR/RID: -

IMDG: -

IATA: -

14.4 Packaging group

ADR/RID: -

IMDG: -

IATA: -

14.5 Environmental hazards

ADR/RID: no

IMDG: no

IATA: no

14.6 Special precautions for user

No data available

15. REGULATORY INFORMATION

This safety datasheet complies with the requirements of Regulations (EU) No. 1907/2006 and No. 1272/2008 and No. 2020/878.

15.1 Safety, health and environmental regulations specific for the substance or mixture

No data available

15.2 Chemical Safety Assessment

For this product no chemical safety assessment was carried out at Enamine Ltd.

16. OTHER INFORMATION

Further information

For R&D use only. Not for drug, household or other uses.

This is an experimental product whose properties are not fully evaluated yet. The information contained herein is based on the present state of our knowledge and therefore does not guarantee certain properties. Recipients of the product must take responsibility for observing existing laws and regulations.

End of Safety Data Sheet