



SAFETY DATA SHEET

Generic SDS - No country specific data

Version 5.8. Revision Date 2021.03.10

Issued on 2023.07.24

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product Name: 2-[3-(1-cyano-1-methylethyl)-5-[(4H-1,2,4-triazol-4-yl)methyl]phenyl]-2-methylpropanenitrile

Product Catalogue Number: EN300-7387412

Number:

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.

CAS-No.: 120511-92-4

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 Chervonotkatska Street02094 KyivUkraine

Telephone: +38 044 495 88 17

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 3), H301

Carcinogenicity(Category 2), H351

Reproductive toxicity(Category 1B), H360

Reproductive toxicity, effects on or via lactation(N/A), H362

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: Danger

Hazard statement(s):

H301 Toxic if swallowed
H351 Suspected of causing cancer
H360 May damage fertility or the unborn child
H362 May cause harm to breast-fed children

Precautionary statements:

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/vapours/spray.
P263 Avoid contact during pregnancy/while nursing.
P264 Wash hands thoroughly after handling. Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P281 Use personal protective equipment as required.
P308+P313 IF exposed or concerned: Get medical advice/attention.
P310 Immediately call a POISON CENTER or doctor/physician.
P330 Rinse mouth.
P405 Store locked up.
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: 2,2'-[5-(4H-1,2,4-TRIAZOL-4-YLMETHYL)-1,3-PHENYLENE]BIS(2-METHYLPROPANENITRILE);2,2'-[5-(4H-1,2,4-TRIAZOL-4-YLMETHYL)-1,3-PHENYLENE]BIS(2-METHYLPROPANENI+

Formula: C17H19N5

Molecular Weight: 293.3663

CAS-No.: 120511-92-4

EC number N/A

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

Component: 2-[3-(1-cyano-1-methylethyl)-5-[(4H-1,2,4-triazol-4-yl)methyl]phenyl]-2-methylpropanenitrile

Classification:

Acute toxicity, oral (Category 3), H301
Carcinogenicity (Category 2), H351
Reproductive toxicity (Category 1B), H360
Reproductive toxicity, effects on or via lactation (N/A), H362

Concentration, %: N/A

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

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 Carbon monoxide, Carbon dioxide, Nitrogen oxides.

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 RT.

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: | powder |
| Odour: | N/A |
| Colour: | lightbrown |
| pH: | N/A |
| Melting point/freezing point (°C): | N/A |
| Initial boiling point and boiling point range (°C): | N/A |
| Flash Point (°C): | N/A |
| Vapour pressure: | N/A |
| Vapour density: | N/A |
| Relative density (g/ml): | |
| Partition coefficient: n-octanol/water: | 0.697 |
| 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: | N/A |

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

Carbon monoxide, Carbon dioxide, Nitrogen oxides

11. TOXICOLOGICAL INFORMATION

N/A

Toxicological properties were not fully evaluated.

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: 2811

IMDG: 2811

IATA: 2811

14.2 UN proper shipping name

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (2-[3-(1-cyano-1-methylethyl)-5-[(4H-1,2,4-triazol-4-yl)methyl]phenyl]-2-methylpropanenitrile)

IMDG: TOXIC SOLID, ORGANIC, N.O.S. (2-[3-(1-cyano-1-methylethyl)-5-[(4H-1,2,4-triazol-4-yl)methyl]phenyl]-2-methylpropanenitrile)

IATA: Toxic solid, organic, n.o.s. (2-[3-(1-cyano-1-methylethyl)-5-[(4h-1,2,4-triazol-4-yl)methyl]phenyl]-2-methylpropanenitrile)

14.3 Transport hazard class(es)

ADR/RID: 6.1

IMDG: 6.1

IATA: 6.1

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

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