

# Safety Data Sheet

**Version:** 01  
**Revision Date:** Aug.-14-2022  
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## 1. PRODUCT AND COMPANY IDENTIFICATION

### 1.1 Product identifier

Product name : (2S,3R)-3-(2,5-Difluorophenyl)-3-hydroxy-2-methyl-4-(1H-1,2,4-triazol-1-yl)butanenitrile  
Catalog No. : CS-Z0013  
CAS No. : 241479-74-3

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

Identified uses : Laboratory chemicals, manufacture of substances.

### 1.3 Details of the supplier of the safety data sheet

Company: ChemScene LLC  
Address: 1 Deer Park Dr, Suite F, Monmouth Junction, NJ 08852, USA  
Tel: 610-426-3128  
Fax: 888-484-5008  
E-mail: sales@chemscene.com

### 1.4 Emergency telephone number

Emergency Phone #: 610-426-3128

## 2. HAZARDS IDENTIFICATION

### 2.1 Classification of the substance or mixture

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

Acute toxicity, oral (Category 4),H302

Skin corrosion/irritation (Category 2),H315

Serious eye damage/eye irritation (Category 2A),H319

Specific target organ toxicity, single exposure; Respiratory tract irritation (Category 3),H335

### 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word Warning

Hazard statement(s)

H302 Harmful if swallowed

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

Precautionary statement(s)

## Prevention

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

## Response

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

## 2.3 Other hazards

None.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

|                   |                                                                                                                               |
|-------------------|-------------------------------------------------------------------------------------------------------------------------------|
| Synonyms:         | ( $\alpha$ S, $\beta$ R)- $\beta$ -(2,5-Difluorophenyl)- $\beta$ -hydroxy- $\alpha$ -methyl-1H-1,2,4-triazole-1-butanenitrile |
| Formula:          | C <sub>13</sub> H <sub>12</sub> F <sub>2</sub> N <sub>4</sub> O                                                               |
| Molecular Weight: | 278.26                                                                                                                        |
| CAS No. :         | 241479-74-3                                                                                                                   |

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### Eye contact

Where Diphoterine is not available, rinse eyes with copious amounts of water for at least 20 minutes. Protect uninjured eye. Remove contact lenses if present and easy to do. Continue rinsing and seek immediate medical attention.

#### Skin contact

Where Diphoterine is not available, wash immediately with plenty of water and soap. Remove contaminated clothing immediately. Immediately seek medical attention.

#### Inhalation

Remove person to fresh air and keep comfortable for breathing. Call a poison centre or physician if you feel unwell. If breathing is irregular or stopped, administer artificial respiration.

#### Ingestion

If accidentally swallowed rinse the mouth with plenty of water (only if the person is conscious) and obtain immediate medical attention. Do not induce vomiting.

### 4.2 Most important symptoms and effects, both acute and delayed

No known symptoms or effects.

### 4.3 Indication of any immediate medical attention and special treatment needed

No special immediate treatment required

## 5. FIRE FIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable fire extinguishing media

Carbon dioxide, alcohol resistant foam or dry chemical powder., Use water to extinguish fire.

#### Unsuitable fire extinguishing media

No known unsuitable media.

### 5.2 Special hazards arising from the substance or mixture

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

### 5.3 Advice for firefighters

Special protective equipment for firefighters : Use personal protective equipment.

Specific extinguishing methods : Use extinguishing measures that are appropriate to local circumstances and the surrounding environment. Immediately evacuate personnel to safe areas. Remove undamaged containers from fire area if it is safe to do so.

## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Keep personnel away from spill/leak.

### 6.2 Environmental precautions

Prevent further leakage if safe to do so. Prevent product from entering drains. Do not let product enter waterways or sewer systems. Discharge into the environment must be avoided.

### 6.3 Methods and materials for containment and cleaning up

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

### 6.4 Reference to other sections

For personal protection see section 8. For disposal see section 13.

## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

#### 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 2.2.

#### Protections against explosions and fire

Where possible, use anti static and spark proof equipment when handling.

#### General occupational hygiene

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. Remove and wash contaminated clothing before re-use.

### 7.2 Conditions for safe storage, including any incompatibilities

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

Recommended storage temperature: Storage temp. 2-8°C

Shipping at room temperature if less than 2 weeks.

### 7.3 Specific end use(s)

No specific end uses are advised. The products supplied are for research purposes only.

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

This product contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### 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 location.

## Personal protective equipment

Eye protection

Safety goggles with side-shields.

Hand protection

Protective gloves.

Skin and body protection

Impervious clothing.

Respiratory protection

Suitable respirator.

Hygiene measures

Ensure hair or skin particles cannot enter the chemical container.

Environment exposure controls

Avoid discharge into the environment, see section 6.2.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

|                                              |                           |
|----------------------------------------------|---------------------------|
| Appearance                                   | Solid                     |
| Odor                                         | No data available         |
| Odor threshold                               | No data available         |
| pH                                           | No data available         |
| Melting/freezing point                       | No data available         |
| Boiling point/range                          | 522.5°C at 760 mmHg       |
| Flash point                                  | 269.8°C                   |
| 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                             | 1.32±0.1g/cm <sup>3</sup> |
| Water Solubility                             | No data available         |
| Partition coefficient                        | No data available         |
| Auto-ignition temperature                    | No data available         |
| Decomposition temperature                    | No data available         |
| Viscosity                                    | No data available         |
| Explosive properties                         | No data available         |
| Oxidizing properties                         | No data available         |

### 9.2 Other safety information

No data available.

## 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

None under normal storage conditions.

### 10.4 Conditions to avoid

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

### 10.5 Incompatible materials

Strong acids/alkalis, strong oxidising/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

No Toxicology data available for this product.

#### Skin corrosion/irritation

No toxicological data available for this product.

#### Serious eye damage/irritation

No toxicological data available for this product.

#### Respiratory or skin sensitisation

No toxicological data available for this product.

#### Germ cell mutagenicity

No toxicological data available for this product.

#### Carcinogenicity

No toxicological data available for this product.

#### Reproductive toxicity

No toxicological data available for this product.

#### Specific target organ toxicity - single exposure

No toxicological data available for this product.

#### Specific target organ toxicity - repeated exposure

No toxicological data available for this product.

#### Aspiration hazard

No toxicological data available for this product.

#### Additional information

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 Ecological data available for this product.

### 12.3 Bioaccumulative potential

No Ecological data available for this product.

### 12.4 Mobility in soil

No Ecological data available for this product.

### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment unavailable 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

Ensure product is disposed of by licensed waste carriers

### 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 (US)

Proper shipping name: Not dangerous goods

UN number: -

Class: -

Packing group: -

### IMDG

Proper shipping name: Not dangerous goods

UN number: -

Class: -

Packing group: -

### IATA

Proper shipping name: Not dangerous goods

UN number: -

Class: -

Packing group: -

## 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:

No SARA Hazards.

### 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 anyother reproductive harm.

## 16. OTHER INFORMATION

Copyright ChemScene. The above information is correct to the best of our present knowledge but does not purport to be all inclusive and should be used only as a guide. The product is for research use only and for experienced personnel. It must only be handled by suitably qualified experienced scientists in appropriately equipped and authorized facilities. The burden of safe use of this material rests entirely with the user. ChemScene disclaims all liability for any damage resulting from handling or from contact with this product.

**Caution: Product has not been fully validated for medical applications. For research use only.**

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