

# 3-(Hydroxymethyl)-4-isopropyl-1-(4-(trifluoromethyl)phenyl)-1H-1,2,4-triazol-5(4H)-one

## Safety Data Sheet 4H563B3

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 02/21/2018 Version: 1.0

### SECTION 1: Identification

#### 1.1. Identification

Product form	: Substance
Substance name	: 3-(Hydroxymethyl)-4-isopropyl-1-(4-(trifluoromethyl)phenyl)-1H-1,2,4-triazol-5(4H)-one
CAS No	: 1050441-89-8
Product code	: 4H56-3-B3
Formula	: C <sub>13</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub>
Other means of identification	: MFCD12923343

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

Use of the substance/mixture	: Laboratory chemicals Manufacture of substances Scientific research and development
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#### 1.3. Details of the supplier of the safety data sheet

SynQuest Laboratories, Inc.  
P.O. Box 309  
Alachua, FL 32615 - United States of America  
T (386) 462-0788 - F (386) 462-7097  
[info@synquestlabs.com](mailto:info@synquestlabs.com) - [www.synquestlabs.com](http://www.synquestlabs.com)

#### 1.4. Emergency telephone number

Emergency number : (844) 523-4086 (3E Company - Account 10069)

### SECTION 2: Hazard(s) identification

#### 2.1. Classification of the substance or mixture

##### Classification (GHS-US)

Skin Irrit. 2 H315 - Causes skin irritation  
Eye Irrit. 2A H319 - Causes serious eye irritation  
STOT SE 3 H335 - May cause respiratory irritation

Full text of H-phrases: see section 16

#### 2.2. Label elements

##### GHS-US labeling

Hazard pictograms (GHS-US) :



GHS07

Signal word (GHS-US) :

Warning

Hazard statements (GHS-US) :

H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation

Precautionary statements (GHS-US) :

P261 - Avoid breathing dust, mist, spray  
P264 - Wash skin thoroughly after handling  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P302+P352 - If on skin: Wash with plenty of soap and water  
P304+P340 - If inhaled: Remove person to fresh air and keep 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+P364 - Take off contaminated clothing and wash it before reuse  
P403+P233 - Store in a well-ventilated place. Keep container tightly closed  
P405 - Store locked up

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P501 - Dispose of contents/container to an approved waste disposal plant

### 2.3. Other hazards

No additional information available

### 2.4. Unknown acute toxicity (GHS US)

Not applicable

## SECTION 3: Composition/information on ingredients

### 3.1. Substance

Substance type : Mono-constituent

Name	Product identifier	%	Classification (GHS-US)
3-(Hydroxymethyl)-4-isopropyl-1-(4-(trifluoromethyl)phenyl)-1H-1,2,4-triazol-5(4H)-one (Main constituent)	(CAS No) 1050441-89-8	<= 100	Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335

Full text of H-phrases: see section 16

### 3.2. Mixture

Not applicable

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

- First-aid measures general : In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Move the affected personnel away from the contaminated area.
- First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing. If not breathing, give artificial respiration. Get medical advice/attention.
- First-aid measures after skin contact : Wash with plenty of soap and water. Get medical advice/attention.
- First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical advice/attention.
- First-aid measures after ingestion : Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get medical advice/attention.

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

- Symptoms/injuries : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

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

Treat symptomatically.

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

- Suitable extinguishing media : Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media appropriate for surrounding fire.

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

- Fire hazard : Thermal decomposition generates: Carbon oxides. Hydrogen fluoride. Nitrogen oxides.

### 5.3. Advice for firefighters

- Firefighting instructions : In case of fire: Evacuate area.
- Protection during firefighting : Wear gas tight chemically protective clothing in combination with self contained breathing apparatus. For further information refer to section 8: "Exposure controls/personal protection".

## SECTION 6: Accidental release measures

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

- General measures : Evacuate unnecessary personnel. Ensure adequate air ventilation. Do not breathe dust.

#### 6.1.1. For non-emergency personnel

- Emergency procedures : Only qualified personnel equipped with suitable protective equipment may intervene.

#### 6.1.2. For emergency responders

- Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".

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### 6.2. Environmental precautions

Avoid release to the environment. Notify authorities if product enters sewers or public waters.

### 6.3. Methods and material for containment and cleaning up

For containment : Stop leak if safe to do so.  
Methods for cleaning up : Sweep or shovel spills into appropriate container for disposal. Minimize generation of dust.  
Other information : For disposal of solid materials or residues refer to section 13 : "Disposal considerations".

### 6.4. Reference to other sections

No additional information available

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

Precautions for safe handling : Do not handle until all safety precautions have been read and understood. Ensure good ventilation of the work station. Do not breathe dust, mist, spray. Wear personal protective equipment. Avoid contact with skin and eyes.  
Hygiene measures : Handle in accordance with good industrial hygiene and safety procedures. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

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

Technical measures : Comply with applicable regulations.  
Storage conditions : Keep container closed when not in use.  
Incompatible materials : Refer to Section 10 on Incompatible Materials.  
Storage area : Store in dry, cool, well-ventilated area.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

No additional information available

### 8.2. Exposure controls

Appropriate engineering controls : Ensure good ventilation of the work station. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.  
Hand protection : Protective gloves. 29 CFR 1910.138: Hand Protection.  
Eye protection : Chemical goggles or safety glasses. Face shield. 29 CFR 1910.133: Eye and Face Protection.  
Skin and body protection : Wear suitable protective clothing.  
Respiratory protection : In case of inadequate ventilation wear respiratory protection. 29 CFR 1910.134: Respiratory Protection.  
Other information : Safety shoes. 29 CFR 1910.136: Foot Protection.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

Physical state : Solid  
Color : No data available  
Odor : No data available  
Odor threshold : No data available  
pH : No data available  
Melting point : No data available  
Freezing point : No data available  
Boiling point : No data available  
Flash point : No data available  
Relative evaporation rate (butyl acetate=1) : No data available  
Flammability (solid, gas) : No data available  
Explosion limits : No data available  
Explosive properties : No data available  
Oxidizing properties : No data available  
Vapor pressure : No data available

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Relative density	: No data available
Relative vapor density at 20 °C	: No data available
Molecular mass	: 301.2644 g/mol
Solubility	: No data available
Log Pow	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available

### 9.2. Other information

No additional information available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

No additional information available

### 10.2. Chemical stability

The product is stable at normal handling and storage conditions.

### 10.3. Possibility of hazardous reactions

No additional information available

### 10.4. Conditions to avoid

Keep away from heat, sparks and flame.

### 10.5. Incompatible materials

Strong oxidizing agents.

### 10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced. Hazardous decomposition products in case of fire, see Section 5.

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity	: Not classified
Skin corrosion/irritation	: Causes skin irritation.
Serious eye damage/irritation	: Causes serious eye irritation.
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
Reproductive toxicity	: Not classified
Specific target organ toxicity (single exposure)	: May cause respiratory irritation.
Specific target organ toxicity (repeated exposure)	: Not classified
Aspiration hazard	: Not classified

## SECTION 12: Ecological information

### 12.1. Toxicity

No additional information available

### 12.2. Persistence and degradability

No additional information available

### 12.3. Bioaccumulative potential

No additional information available

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### 12.4. Mobility in soil

No additional information available

### 12.5. Other adverse effects

No additional information available

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

Waste treatment methods : Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.  
Waste disposal recommendations : Dispose of contents/container in accordance with licensed collector's sorting instructions.  
Additional information : Recycle the material as far as possible.

## SECTION 14: Transport information

### Department of Transportation (DOT)

In accordance with DOT  
Not regulated for transport

### TDG

No additional information available

### Transport by sea

No additional information available

### Air transport

No additional information available

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

All components of this product are listed, or excluded from listing, on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory except for:

3-(Hydroxymethyl)-4-isopropyl-1-(4-(trifluoromethyl)phenyl)-1H-1,2,4-triazol-5(4H)-one	CAS No 1050441-89-8	100%
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This product or mixture does not contain a toxic chemical or chemicals in excess of the applicable de minimis concentration as specified in 40 CFR §372.38(a) subject to the reporting requirements of section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 and 40 CFR Part 372.

### 15.2. International regulations

#### CANADA

No additional information available

#### EU-Regulations

No additional information available

#### National regulations

No additional information available

### 15.3. US State regulations

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer and/or reproductive harm

## SECTION 16: Other information

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### Full text of H-phrases:

Eye Irrit. 2A	Serious eye damage/eye irritation Category 2A
Skin Irrit. 2	Skin corrosion/irritation Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H315	Causes skin irritation
H319	Causes serious eye irritation
H335	May cause respiratory irritation

### NFPA health hazard

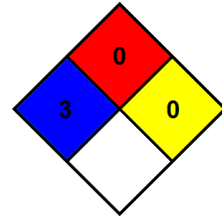
: 3 - Short exposure could cause serious temporary or residual injury even though prompt medical attention was given.

### NFPA fire hazard

: 0 - Materials that will not burn.

### NFPA reactivity

: 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



### HMIS III Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur  
Flammability : 0 Minimal Hazard - Materials that will not burn  
Physical : 0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

### SDS US (GHS HazCom 2012)

*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 offered solely for your consideration, investigation, and verification. It does not represent any guarantee of the properties of the product nor that the hazard precautions or procedures described are the only ones which exist. SynQuest shall not be held liable or any damage resulting from handling or from contact with the above product.*