

# 2-[1-Methyl-5-(trifluoromethyl)-1H-pyrazol-3-yl]thiophene-5-sulfonyl chloride

## Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations  
 SDS ID: 8H627X1  
 Issue date: 8/22/2023 Version: 1.0

### SECTION 1: Identification

#### 1.1. Identification

Product form : Substance  
 Substance name : 2-[1-Methyl-5-(trifluoromethyl)-1H-pyrazol-3-yl]thiophene-5-sulfonyl chloride  
 CAS-No. : 166964-31-4  
 Product code : 8H62-7-X1  
 Formula : C<sub>9</sub>H<sub>6</sub>ClF<sub>3</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>  
 Other means of identification : MFCD00052283

#### 1.2. Recommended use and restrictions on use

Use of the substance/mixture : Laboratory chemicals  
 Manufacture of substances  
 Scientific research and development

#### 1.3. Supplier

SynQuest Laboratories, Inc. Inc.  
 P.O. Box 309  
 Alachua, FL, Alachua, 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

##### GHS US classification

Corrosive to metals Category 1	H290	May be corrosive to metals
Skin corrosion/irritation Category 1B	H314	Causes severe skin burns and eye damage
Serious eye damage/eye irritation Category 1	H318	Causes serious eye damage
Specific target organ toxicity – Single exposure, Category 3, Respiratory tract irritation	H335	May cause respiratory irritation

Full text of H statements : see section 16

#### 2.2. GHS Label elements, including precautionary statements

##### GHS US labeling

Hazard pictograms (GHS US) : 

Signal word (GHS US) : Danger  
 Hazard statements (GHS US) : H290 - May be corrosive to metals  
 H314 - Causes severe skin burns and eye damage  
 H318 - Causes serious eye damage  
 H335 - May cause respiratory irritation

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Precautionary statements (GHS US) : P234 - Keep only in original container.  
P260 - Do not breathe 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.  
P301+P330+P331 - If swallowed: rinse mouth. Do NOT induce vomiting.  
P303+P361+P353 - If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.  
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.  
P310 - Immediately call a POISON CENTER or doctor/ physician  
P321 - Specific treatment (see supplemental first aid instructions on this label)  
P363 - Wash contaminated clothing before reuse.  
P390 - Absorb spillage to prevent material-damage.  
P403+P233 - Store in a well-ventilated place. Keep container tightly closed.  
P405 - Store locked up.  
P406 - Store in corrosive resistant container with a resistant inner liner  
P501 - Dispose of contents/container to an approved waste disposal plant

### 2.3. Other hazards which do not result in classification

Other hazards which do not result in classification : Stench.

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

No additional information available

## SECTION 3: Composition/Information on ingredients

### 3.1. Substances

Substance type : Mono-constituent

Name	Product identifier	%	GHS US classification
2-[1-Methyl-5-(trifluoromethyl)-1H-pyrazol-3-yl]thiophene-5-sulfonyl chloride (Main constituent)	CAS-No.: 166964-31-4	≤ 100	Met. Corr. 1, H290 Skin Corr. 1B, H314 Eye Dam. 1, H318 STOT SE 3, H335

Full text of hazard classes and H-statements : see section 16

### 3.2. Mixtures

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 immediate medical advice/attention.  
First-aid measures after skin contact : Wash with plenty of soap and water. Remove contaminated clothing and shoes. Get immediate medical advice/attention.

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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 immediate 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 immediate medical advice/attention.

### 4.2. Most important symptoms and effects (acute and delayed)

Symptoms/effects	: The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.
Symptoms/effects after inhalation	: Material is destructive to tissue of the mucuous membranes and upper respiratory tract. Cough, shortness of breath, headache, nausea.

### 4.3. Immediate medical attention and special treatment, if necessary

Treat symptomatically.

## SECTION 5: Fire-fighting measures

### 5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media	: The product itself does not burn. Use extinguishing media appropriate for surrounding fire.
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### 5.2. Specific hazards arising from the chemical

Fire hazard	: Thermal decomposition generates: Carbon oxides. Hydrogen chloride. Hydrogen fluoride. Nitrogen oxides. Sulfur oxides.
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### 5.3. Special protective equipment and precautions for fire-fighters

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.
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#### 6.1.1. For non-emergency personnel

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

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### 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. Moisture sensitive. Keep contents under inert gas.
- 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

##### 2-[1-Methyl-5-(trifluoromethyl)-1H-pyrazol-3-yl]thiophene-5-sulfonyl chloride (166964-31-4)

No additional information available

#### 8.2. Appropriate engineering 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.

#### 8.3. Individual protection measures/Personal protective equipment

##### 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

#### Personal protective equipment symbol(s):



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### 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	: Stench
Odor threshold	: No data available
pH	: No data available
Melting point	: 77 – 80 °C
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
Vapor pressure	: No data available
Relative vapor density at 20 °C	: No data available
Relative density	: No data available
Molecular mass	: 330.72 g/mol
Solubility	: No data available
Partition coefficient n-octanol/water (Log Pow)	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosion limits	: No data available
Explosive properties	: No data available
Oxidizing properties	: 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.

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### 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 (oral)	: Not classified
Acute toxicity (dermal)	: Not classified
Acute toxicity (inhalation)	: Not classified
Skin corrosion/irritation	: Causes severe skin burns.
Serious eye damage/irritation	: Causes serious eye damage.
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
Reproductive toxicity	: Not classified
STOT-single exposure	: May cause respiratory irritation.
STOT-repeated exposure	: Not classified
Aspiration hazard	: Not classified
Viscosity, kinematic	: No data available
Symptoms/effects	: The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.
Symptoms/effects after inhalation	: Material is destructive to tissue of the mucuous membranes and upper respiratory tract. Cough, shortness of breath, headache, nausea.

## 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

### 12.4. Mobility in soil

No additional information available

### 12.5. Other adverse effects

No additional information available

## SECTION 13: Disposal considerations

### 13.1. Disposal methods

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

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### SECTION 14: Transport information

#### 14.1. UN number

DOT NA No : UN1759  
UN-No. (TDG) : UN1759  
UN-No. (IMDG) : 1759  
UN-No. (IATA) : 1759

#### 14.2. UN proper shipping name

Proper Shipping Name (DOT) : Corrosive solids, n.o.s.  
Proper Shipping Name (TDG) : CORROSIVE SOLID, N.O.S.  
Proper Shipping Name (IMDG) : CORROSIVE SOLID, N.O.S.  
Proper Shipping Name (IATA) : Corrosive solid, n.o.s.

#### 14.3. Transport hazard class(es)

##### DOT

Transport hazard class(es) (DOT) : 8  
Hazard labels (DOT) : 8



##### TDG

Transport hazard class(es) (TDG) : 8  
Hazard labels (TDG) : 8



##### IMDG

Transport hazard class(es) (IMDG) : 8  
Hazard labels (IMDG) : 8



##### IATA

Transport hazard class(es) (IATA) : 8  
Hazard labels (IATA) : 8



#### 14.4. Packing group

Packing group (DOT) : III  
Packing group (TDG) : III  
Packing group (IMDG) : III

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Packing group (IATA) : III

### 14.5. Environmental hazards

Other information : No supplementary information available.

### 14.6. Special precautions for user

#### DOT

UN-No.(DOT) : UN1759

DOT Special Provisions (49 CFR 172.102) : 128 - Regardless of the provisions of §172.101(c)(12), aluminum smelting by-products and aluminum remelting by-products described under this entry, meeting the definition of Class 8, Packing Group II and III may be classed as a Division 4.3 material and transported under this entry. The presence of a Class 8 hazard must be communicated as required by this Part for subsidiary hazards

IB8 - Authorized IBCs: Metal (11A, 11B, 11N, 21A, 21B, 21N, 31A, 31B and 31N); Rigid plastics (11H1, 11H2, 21H1, 21H2, 31H1 and 31H2); Composite (11HZ1, 11HZ2, 21HZ1, 21HZ2, 31HZ1 and 31HZ2); Fiberboard (11G); Wooden (11C, 11D and 11F); Flexible (13H1, 13H2, 13H3, 13H4, 13H5, 13L1, 13L2, 13L3, 13L4, 13M1 or 13M2).

IP3 - Flexible IBCs must be sift-proof and water-resistant or must be fitted with a sift-proof and water-resistant liner.

T1 - 1.5 178.274(d)(2) Normal..... 178.275(d)(2)

TP33 - The portable tank instruction assigned for this substance applies for granular and powdered solids and for solids which are filled and discharged at temperatures above their melting point which are cooled and transported as a solid mass. Solid substances transported or offered for transport above their melting point are authorized for transportation in portable tanks conforming to the provisions of portable tank instruction T4 for solid substances of packing group III or T7 for solid substances of packing group II, unless a tank with more stringent requirements for minimum shell thickness, maximum allowable working pressure, pressure-relief devices or bottom outlets are assigned in which case the more stringent tank instruction and special provisions shall apply. Filling limits must be in accordance with portable tank special provision TP3. Solids meeting the definition of an elevated temperature material must be transported in accordance with the applicable requirements of this subchapter.

DOT Packaging Exceptions (49 CFR 173.xxx) : 154

DOT Packaging Non Bulk (49 CFR 173.xxx) : 213

DOT Packaging Bulk (49 CFR 173.xxx) : 240

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 25 kg

DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 100 kg

DOT Vessel Stowage Location : A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.

#### TDG

UN-No. (TDG) : UN1759

TDG Special Provisions : 16 - 1) The technical name of the most dangerous substance related to the primary class must be shown, in parentheses, on the shipping document following the shipping name in accordance with clause 3.5(1)(c)(i)(A) of Part 3, Documentation. The technical name must also be shown, in parentheses, on a small means of containment or on a tag following the shipping name in accordance with subsections 4.11(2) and (3) of Part 4, Dangerous Goods Safety Marks. 2) subsection (1), the technical name for the following dangerous goods is not required to be shown on a shipping document or on a small means of containment when Canadian law for domestic transport or an international convention for international transport prohibits the disclosure of the technical: a) UN1544, ALKALOID SALTS, SOLID, N.O.S. or ALKALOIDS, SOLID, N.O.S; b) UN1851, MEDICINE, LIQUID, TOXIC, N.O.S; c) UN3140, ALKALOID SALTS, LIQUID, N.O.S. or ALKALOIDS, LIQUID, N.O.S; d) UN3248, MEDICINE, LIQUID, FLAMMABLE, TOXIC, N.O.S; or e) UN3249, MEDICINE, SOLID, TOXIC, N.O.S. An example in Canada is the "Food and Drugs Act".



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Explosive Limit and Limited Quantity Index : 5 kg  
Excepted quantities (TDG) : E1  
Passenger Carrying Road Vehicle or Passenger Carrying Railway Vehicle Index : 25 kg  
Emergency Response Guide (ERG) Number : 154

### IMDG

Special provision (IMDG) : 223, 274  
Limited quantities (IMDG) : 5 kg  
Excepted quantities (IMDG) : E1  
Packing instructions (IMDG) : P002, LP02  
IBC packing instructions (IMDG) : IBC08  
IBC special provisions (IMDG) : B3  
Tank instructions (IMDG) : T1  
Tank special provisions (IMDG) : TP33  
EmS-No. (Fire) : F-A - FIRE SCHEDULE Alfa - GENERAL FIRE SCHEDULE  
EmS-No. (Spillage) : S-B - SPILLAGE SCHEDULE Bravo - CORROSIVE SUBSTANCES  
Stowage category (IMDG) : A  
Properties and observations (IMDG) : Causes burns to skin, eyes and mucous membranes.

### IATA

PCA Excepted quantities (IATA) : E1  
PCA Limited quantities (IATA) : Y845  
PCA limited quantity max net quantity (IATA) : 5kg  
PCA packing instructions (IATA) : 860  
PCA max net quantity (IATA) : 25kg  
CAO packing instructions (IATA) : 864  
CAO max net quantity (IATA) : 100kg  
Special provision (IATA) : A3, A803  
ERG code (IATA) : 8L

### 14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

All components of this product are present and listed as Active on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory, except for:

2-[1-Methyl-5-(trifluoromethyl)-1H-pyrazol-3-yl]thiophene-5-sulfonyl chloride	CAS-No. 166964-31-4	100%
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### 15.2. International regulations

#### CANADA

No additional information available

#### EU-Regulations

No additional information available

#### National regulations

No additional information available

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### 15.3. US State regulations

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

### SECTION 16: Other information

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Full text of H-phrases	
H290	May be corrosive to metals
H314	Causes severe skin burns and eye damage
H318	Causes serious eye damage
H335	May cause respiratory irritation

NFPA health hazard

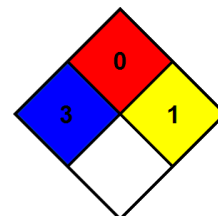
: 3 - Materials that, under emergency conditions, can cause serious or permanent injury.

NFPA fire hazard

: 0 - Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand.

NFPA reactivity

: 1 - Materials that in themselves are normally stable but can become unstable at elevated temperatures and pressures.



Hazard Rating

Health : 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given

Flammability : 0 Minimal Hazard - Materials that will not burn

Physical : 1 Slight Hazard - Materials that are normally stable but can become unstable (self-react) at high temperatures and pressures. Materials may react non-violently with water or undergo hazardous polymerization in the absence of inhibitors.

Safety Data Sheet (SDS), USA

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.