

1-(4-Fluorophenyl)-2-(2-(methylthio)pyrimidin-4-yl)ethanone

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
 SDS ID: 8H6632A
 Issue date: 1/2/2025 Version: 1.0

SECTION 1: Identification

1.1. Identification

Product form : Substance
 Substance name : 1-(4-Fluorophenyl)-2-(2-(methylthio)pyrimidin-4-yl)ethanone
 CAS-No. : 217661-99-9
 Product code : 8H66-3-2A
 Formula : C13H11FN2OS
 Other means of identification : MFCD18157689

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.
 P.O. Box 309
 Alachua, FL, Alachua, 32615
 United States of America
 T (386) 462-0788 - F (386) 462-7097
info@synquestlabs.com - 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

Skin corrosion/irritation Category 2	H315	Causes skin irritation
Serious eye damage/eye irritation Category 1	H318	Causes serious eye damage
Skin sensitization, Category 1	H317	May cause an allergic skin reaction
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) : H315 - Causes skin irritation
 H317 - May cause an allergic skin reaction
 H318 - Causes serious eye damage
 H335 - May cause respiratory irritation

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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.
P272 - Contaminated work clothing must not be allowed out of the workplace.
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.
P310 - Immediately call a POISON CENTER or doctor/ physician
P321 - Specific treatment (see supplemental first aid instructions on this label)
P332+P313 - If skin irritation occurs: Get medical advice/attention.
P333+P313 - If skin irritation or rash occurs: Get medical advice/attention.
P362+P364 - Take off contaminated clothing and wash it before reuse.
P363 - Wash contaminated clothing before reuse.
P403+P233 - Store in a well-ventilated place. Keep container tightly closed.
P405 - Store locked up.
P501 - Dispose of contents/container to an approved waste disposal plant

2.3. Other hazards which do not result in classification

No additional information available

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
1-(4-Fluorophenyl)-2-(2-(methylthio)pyrimidin-4-yl)ethanone (Main constituent)	CAS-No.: 217661-99-9	≤ 100	Skin Irrit. 2, H315 Eye Dam. 1, H318 Skin Sens. 1, H317 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 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.

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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.

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

5.2. Specific hazards arising from the chemical

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

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.

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".

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.
- 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. 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):



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

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Color	: No data available
Odor	: No data available
Odor threshold	: No data available
pH	: No data available
Melting point	: 88 – 90 °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	: 262.3 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 acids. 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 (oral) : Not classified

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Acute toxicity (dermal)	: Not classified
Acute toxicity (inhalation)	: Not classified
Skin corrosion/irritation	: Causes skin irritation.
Serious eye damage/irritation	: Causes serious eye damage.
Respiratory or skin sensitization	: May cause an allergic skin reaction.
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.

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

12.2. Persistence and degradability

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Persistence and degradability	Rapidly degradable
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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.

SECTION 14: Transport information

14.1. UN number

DOT NA No	: Not applicable
UN-No. (TDG)	: Not applicable
UN-No. (IMDG)	: Not applicable
UN-No. (IATA)	: Not applicable

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14.2. UN proper shipping name

Proper Shipping Name (DOT) : Not applicable
Proper Shipping Name (TDG) : Not applicable
Proper Shipping Name (IMDG) : Not applicable
Proper Shipping Name (IATA) : Not applicable

14.3. Transport hazard class(es)

DOT
Transport hazard class(es) (DOT) : Not applicable

TDG
Transport hazard class(es) (TDG) : Not applicable

IMDG
Transport hazard class(es) (IMDG) : Not applicable

IATA
Transport hazard class(es) (IATA) : Not applicable

14.4. Packing group

Packing group (DOT) : Not applicable
Packing group (TDG) : Not applicable
Packing group (IMDG) : Not applicable
Packing group (IATA) : Not applicable

14.5. Environmental hazards

Other information : No supplementary information available.

14.6. Special precautions for user

DOT
Not applicable

TDG
Not applicable

IMDG
Not applicable

IATA
Not applicable

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:

1-(4-Fluorophenyl)-2-(2-(methylthio)pyrimidin-4-yl)ethanone	CAS-No. 217661-99-9	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

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	
H315	Causes skin irritation
H317	May cause an allergic skin reaction
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.

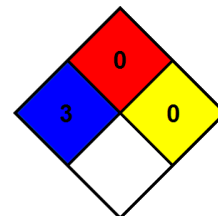
NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.

Hazard 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.



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.