

Safety Data Sheet

fluorochem.

1. Identification of the substance/mixture

1.1 Product identification

Product name	8-Bromo-7-(but-2-yn-1-yl)-3-methyl-1-((4-methylquinazolin-2-yl)methyl)-1H-purine-2,6(3H,7H)-dione
Other names	
Product code	F789950
CAS	853029-57-9
MDL	MFCD18642578
EINECS	N/A
REACH Registration number	N/A
Nanoform	The product does not contain nanoparticles.

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

Relevant uses	For research and development purposes.
Uses advised against	No uses advised.

1.3 Safety Data Sheet supplier details

Company	Fluorochem Limited
Address	Unit 14, Graphite Way Hadfield Glossop Derbys. SK13 1QH United Kingdom
Telephone	+44 1457 860111
Email	sds@fluorochem.co.uk

1.4 Emergency Telephone

Emergency Telephone	+44 20 3807 3798 (Poison Information)
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2. Hazard Identification

2.1 Classification of the substance or mixture

Classification	H302 Acute Tox. 4 H315 Skin Irrit. 2 H319 Eye Irrit. 2 H335 STOT SE 3
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2.2 Label Elements

Signal Word

Warning

Pictograms



GHS07

Hazards

H302 Harmful if swallowed.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.

Precautions

P101 If medical advice is needed, have product container or label at hand.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P280 Wear protective gloves/protective clothing and eye/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.
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.
P321 Specific treatment (see Section 4 on this SDS).
P405 Store locked up.
P501 Dispose of contents/container to hazardous waste disposal.

Supplemental Hazard Information

None

2.3 Other Hazards

Other Classification Hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological Information

This substance/mixture contains no components considered to have endocrine disrupting properties for environment, according to REACH Article 57(f), Commission Regulation (EU) 2018/605 or Commission Delegated Regulation (EU) 2017/2100.

Toxicological Information

This substance/mixture contains no components considered to have endocrine disrupting properties affecting human health, according to REACH Article 57(f), Commission Regulation (EU) 2018/605 or Commission Delegated Regulation (EU) 2017/2100.

3. Composition

3.1 SUBSTANCE

Name	CAS	Einecs	Composition	Hazards
8-Bromo-7-(but-2-yn-1-yl)-3-methyl-1-((4-methylquinazolin-2-yl)methyl)-1H-purine-2,6(3H,7H)-dione	853029-57-9	N/A		H302 Acute Tox. 4 H315 Skin Irrit. 2 H319 Eye Irrit. 2 H335 STOT SE 3

3.2 MIXTURE

Not applicable. Product is a substance.

For the full text of the H-Statements mentioned in this Section, see Section 16.

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.
Ingestion	Where Diphoterine is not available, rinse mouth with copious amounts of water. Seek urgent medical advice.
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.
Skin Contact	Where Diphoterine is not available, wash immediately with plenty of water and soap. Remove contaminated clothing immediately. Immediately seek medical attention.
General Advice	If exposed or concerned, seek immediate medical attention.

4.2 Most Important Symptoms and Effects

Most Important Symptoms and Effects	No known symptoms or effects.
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4.3 Indication of any urgent medical attention and special treatments needed

Immediate First Aid Measures	No special immediate treatment required.
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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

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

5.3 Recommendations for firefighting personnel

Advice for Fire Fighters As in any fire, wear self-contained breathing apparatus and full protective gear.

6. Accidental Release Measures

6.1 Personal precautions, protective equipment and emergency procedures

Personal precautions 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

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 Containment and cleaning methods and materials

Containment - Methods and Materials 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 References to other sections

Referenced SDS 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.

Protection Against Explosion 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 and Incompatibilities

Managing Storage Risks	Keep container tightly closed and upright. Store in a cool, dry and well-ventilated place
Storage Controls	No special requirements
Maintaining Integrity	Keep container tightly closed in a cool area away from sunlight or heat sources
Storage Class	Storage class (TRGS 510): 13, Non-combustible solids
Other Advice	No other specific advice available

7.3 Specific End Use(s)

Specific End Use(s)	No specific end uses are advised. The products supplied are for research purposes only.
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8. Exposure Controls / Personal Protection

8.1 Control Parameters

Control Parameters	No data available.
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8.2 Exposure Controls

Engineering Measures	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.
Face Protection	Wear tightly fitting safety goggles which adhere to European standard EN 166. Ensure eye bath is to hand.
Hand Protection	Handle with impermeable gloves. Inspect gloves before use. Gloves must satisfy the specifications of EU Directive 89/686/EEC and the standard EN374 derived from it. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.
Skin Protection	Wear appropriate protective clothing ensuring all skin is covered. Wear safety shoes that meet at least S1 standards. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.
Respiratory Protection	Product should be handled in a fume cupboard with adequate extraction. No respiratory equipment is needed under normal use conditions.
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

a) State	No data available.
b) Colour	No data available.
c) Odour	No data available.
d) Melting Point / Freezing Point	No data available.
e) Initial Boiling point or Boiling range	No data available.
f) Flammability	No data available.
g) Upper / Lower Flammability or Explosion Limits	No data available.
h) Flash Point	No data available.
i) Auto Ignition Temperature	No data available.
j) Decomposition Temperature	No data available.
k) pH	No data available.
l) Viscosity	No data available.
m) Solubility	No data available.
n) Partition Coefficient	No data available.
o) Vapour Pressure	No data available.
p) Relative Density	No data available.
q) Vapour Density	No data available.
r) Appearance	No data available.

9.2 Other Safety Information

Other Information No data available.

10. Stability and Reactivity

10.1 Reactivity

Reactivity No data available.

10.2 Stability

Stability Stable under recommended storage conditions.

10.3 Possibility of Hazardous Reactions

Possibility of Hazardous Reactions None under normal storage conditions.

10.4 Conditions to Avoid

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

10.5 Incompatible Materials

Incompatible Materials Strong oxidizing agents.

10.6 Hazardous Decomposition Products

Hazardous Decomposition Products No data available.

11. Toxicology Information

11.1 Information on Hazard Classes, as defined in Regulation (EC) No. 1271/2008

Acute Toxicity	No toxicological data available for this product.
Skin Corrosion / Irritation	No Toxicology data available for this product.
Serious Eye Damage / Irritation	No Toxicology data available for this product.
Respiratory or Skin Sensitisation	No Toxicology data available for this product.
Germ Cell Mutagenicity	No Toxicology data available for this product.
Carcinogenicity	No Toxicology data available for this product.
Reproductive Toxicity	No Toxicology data available for this product.
STOT-single Exposure	No Toxicology data available for this product.
STOT-repeated Exposure	No Toxicology data available for this product.
Aspiration Hazard	No Toxicology data available for this product.

11.2 Information about Other Hazards

Addition Toxicology Information	No Toxicology data available for this product.
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12. Ecological Information

12.1 Toxicity

Toxicity	No Ecological data available for this product.
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12.2 Persistence and Degradability

Persistence and Degradability	No Ecological data available for this product.
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12.3 Bio-Accumulative Potential

Bio-Accumulative Potential	No Ecological data available for this product.
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12.4 Mobility in Soil

Mobility in Soil	No Ecological data available for this product.
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12.5 Results of PBT and vPvB assessment

Results of PBT and vPvB assessment	This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.
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12.6 Endocrine Disrupting Properties

Endocrine Disrupting Properties	No Ecological data available for this product.
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12.7 Other Adverse Effects

Other Adverse Effects Avoid release to the environment.

13. Disposal Considerations

13.1 Waste Treatment Methods

Disposal Operations Ensure product is disposed of by licensed waste carriers.
Disposal of Packaging Ensure INNER PACKAGING is disposed of by licensed waste carriers. Some OUTER PACKAGING MAY be recyclable if not contaminated.

14. Transport Information

14.1 UN Number

IATA UN Number	No data available.	ADR UN Number	No data available.	IMDG UN Number	No data available.
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14.2 Official UN Shipping Name

IATA Proper Shipping Name	Non Hazardous For Transport (8-Bromo-7-(but-2-yn-1-yl)-3-methyl-1-((4-methylquinazolin-2-yl)methyl)-1H-purine-2,6(3H,7H)-dione)	ADR Proper Shipping Name	Non Hazardous For Transport (8-Bromo-7-(but-2-yn-1-yl)-3-methyl-1-((4-methylquinazolin-2-yl)methyl)-1H-purine-2,6(3H,7H)-dione)	IMDG Proper Shipping Name	Non Hazardous For Transport (8-Bromo-7-(but-2-yn-1-yl)-3-methyl-1-((4-methylquinazolin-2-yl)methyl)-1H-purine-2,6(3H,7H)-dione)
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14.3 Hazard classes for transport purposes

IATA Hazard Class	No data available.	ADR Hazard Class	No data available.	IMDG Hazard Class	No data available.
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14.4 Packing Group

IATA Packing Group	No data available.	ADR Packing Group	No data available.	IMDG Packing Group	No data available.
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14.5 Environmental Hazards

IATA Environmental Hazards	No data available.	ADR Environmental Hazards	No data available.	IMDG Environmental Hazards	No data available.
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14.6 Special Precautions

No Information Available

14.7 Bulk Maritime Transport in accordance with IMO Instructions

IATA Sub Class	No data available.	ADR Sub Class	No data available.	IMDG Sub Class	No data available.
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15. Regulatory Information

15.1 Health, safety and environmental regulations/legislation specific to the substance or mixture

Regulatory Information	This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.
Authorisations and Restrictions on Use	REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII): Entry Number:3
National Legislation	Water contaminating class (Germany): WGK 3, highly hazardous to water - Self Classification, Classification according to AwSV, Annex 1 (4)

15.2 Chemical Safety Assessment

Chemical Safety Assessment	There is no chemical safety assessment available for this product.
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16. Other Information

Information Not Covered in Other Sections

Full Text of H-Statements

H302 Harmful if swallowed.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.

Full Text of Abbreviations

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road (European agreement on the international transport of dangerous goods by road)
CAS: Chemical Abstracts Service
EC50: Effective Concentration 50%
EINECS: European Inventory of Existing Commercial Chemical Substances
ErC50: Effective Reduction Concentration in Growth Rate 50%
GHS: Globally Harmonized System for Classification and Labelling of Chemicals
IATA-DGR: Dangerous Goods Regulations for International Air Transport Association
IATA: International Air Transport Association
ICAO-TI: Technical instructions from ICAO
ICAO: International Civil Aviation Organisation
IMDG: International Maritime Code for Dangerous Goods
LC50: Lethal Concentration 50%
LCLo: Lethal Concentration Low
LD50: Lethal Dose 50%
MDL: Molecular Data Library
PBT: Persistent, Bioaccumulative and Toxic substance
REACH: Registration, Evaluation, Authorisation and Restriction of Chemicals
RID: International Regulations concerning the Transport of Dangerous Goods by Rail (Regulations regarding the international transport of dangerous goods by rail)
SDS: Safety Data Sheet
STOT: Specific target organ toxicity
vPvB: Very Persistent and Very Bioaccumulative
WEL: Workplace Exposure Limit

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Other Information

Changes From Previous Version

Changes From Previous Version

1. Other Information

Disclaimer

The product listed is for research and development purposes only and not for human or animal use. As such, in most cases, the toxicological, ecological and physico-chemical properties have not been fully determined and the product should be treated with respect and always handled under suitable conditions by appropriately qualified personnel. The responsible party shall use this datasheet only in conjunction with other sources of information gathered by them, and should make an independent judgement of suitability, to ensure proper use and protect the health and safety of employees. This informat-

In compliance with the regulation (CE) no. 1907/2006

ion is furnished without warranty and any use of the product not in conformance with this material safety data sheet, or in combination with any other product or process, is the responsibility of the user. This SDS adheres to Regulation (EC) No 1907/2006, and as of 13th April 2023, also conforms to EU Regulation 2020/878.