

# Safety Data Sheet

fluorochem.

## 1. Identification of the substance/mixture

### 1.1 Product identification

Product name	(5S)-(1R,2S,5R)-2-ISOPROPYL-5-METHYLCYCLOHEXYL 5-(4-AMINO-5-FLUORO-2-OXOPYRIMIDIN-1(2H)-YL)-1,3-OXATHIOLANE-2-CARBOXYLATE
Other names	
Product code	F475066
CAS	764659-79-2
MDL	MFCD27978447
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
(5S)- (1R,2S,5R)-2- ISOPROPYL-5- METHYLCYCL OHEXYL 5-(4- AMINO-5- FLUORO-2- OXOPYRIMIDI N-1(2H)- YL)-1,3- OXATHIOLANE -2- CARBOXYLAT E	764659-79-2	N/A		<b>H302</b> Acute Tox. 4 <b>H315</b> Skin Irrit. 2 <b>H319</b> Eye Irrit. 2 <b>H335</b> 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

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

### 4.2 Most Important Symptoms and Effects

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

<b>Immediate First Aid Measures</b>	No special immediate treatment required.
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## 5. Fire Fighting Measures

### 5.1 Extinguishing Media

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

**Unsuitable Fire Extinguishing Media** No known unsuitable media.

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

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

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## **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.

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## **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.

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## **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.

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## **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.

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## 7.2 Conditions for Safe Storage and Incompatibilities

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

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## 7.3 Specific End Use(s)

<b>Specific End Use(s)</b>	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

<b>Control Parameters</b>	No data available.
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## 8.2 Exposure Controls

<b>Engineering Measures</b>	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.
<b>Face Protection</b>	Wear tightly fitting safety goggles which adhere to European standard EN 166. Ensure eye bath is to hand.
<b>Hand Protection</b>	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.
<b>Skin Protection</b>	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.
<b>Respiratory Protection</b>	Product should be handled in a fume cupboard with adequate extraction. No respiratory equipment is needed under normal use conditions.
<b>Hygiene Measures</b>	Ensure hair or skin particles cannot enter the chemical container.
<b>Environment Exposure Controls</b>	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.

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### 9.2 Other Safety Information

Other Information	No data available.
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## 10. Stability and Reactivity

### 10.1 Reactivity

Reactivity	No data available.
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### 10.2 Stability

Stability	Stable under recommended storage conditions.
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### 10.3 Possibility of Hazardous Reactions

Possibility of Hazardous Reactions	None under normal storage conditions.
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### 10.4 Conditions to Avoid

<b>Conditions to Avoid</b>	Heat, sparks, open flames, sources of ignition. Exposure to moisture.
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### **10.5 Incompatible Materials**

<b>Incompatible Materials</b>	Strong oxidizing agents.
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### **10.6 Hazardous Decomposition Products**

<b>Hazardous Decomposition Products</b>	No data available.
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## **11. Toxicology Information**

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

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

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### **11.2 Information about Other Hazards**

<b>Addition Toxicology Information</b>	No Toxicology data available for this product.
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## **12. Ecological Information**

### **12.1 Toxicity**

<b>Toxicity</b>	No Ecological data available for this product.
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### **12.2 Persistence and Degradability**

<b>Persistence and Degradability</b>	No Ecological data available for this product.
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### **12.3 Bio-Accumulative Potential**

<b>Bio-Accumulative Potential</b>	No Ecological data available for this product.
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### **12.4 Mobility in Soil**

<b>Mobility in Soil</b>	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.

## 12.6 Endocrine Disrupting Properties

**Endocrine Disrupting Properties** No Ecological data available for this product.

## 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

<b>IATA UN Number</b>	No data available.	<b>ADR UN Number</b>	No data available.	<b>IMDG UN Number</b>	No data available.
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## 14.2 Official UN Shipping Name

<b>IATA Proper Shipping Name</b>	((5S)-(1R,2S,5R)-2-ISOPROPYL-5-METHYLCYCLOHEXYL 5-(4-AMINO-5-FLUORO-2-OXOPYRIMIDIN-1(2H)-YL)-1,3-OXATHIOLANE-2-CARBOXYLATE)	<b>ADR Proper Shipping Name</b>	Non Hazardous For Transport ((5S)-(1R,2S,5R)-2-ISOPROPYL-5-METHYLCYCLOHEXYL 5-(4-AMINO-5-FLUORO-2-OXOPYRIMIDIN-1(2H)-YL)-1,3-OXATHIOLANE-2-CARBOXYLATE)	<b>IMDG Proper Shipping Name</b>	((5S)-(1R,2S,5R)-2-ISOPROPYL-5-METHYLCYCLOHEXYL 5-(4-AMINO-5-FLUORO-2-OXOPYRIMIDIN-1(2H)-YL)-1,3-OXATHIOLANE-2-CARBOXYLATE)
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## 14.3 Hazard classes for transport purposes

<b>IATA Hazard Class</b>	No data available.	<b>ADR Hazard</b>
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<b>Class</b>	No data available.	<b>IMDG Hazard Class</b>	No data available.
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### **14.4 Packing Group**

<b>IATA Packing Group</b>	No data available.	<b>ADR Packing Group</b>	No data available.	<b>IMDG Packing Group</b>	No data available.
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### **14.5 Environmental Hazards**

<b>IATA Environmental Hazards</b>	No data available.	<b>ADR Environmental Hazards</b>	No data available.	<b>IMDG Environmental Hazards</b>	No data available.
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### **14.6 Special Precautions**

No Information Available

### **14.7 Bulk Maritime Transport in accordance with IMO Instructions**

<b>IATA Sub Class</b>	No data available.	<b>ADR Sub Class</b>	No data available.	<b>IMDG Sub Class</b>	No data available.
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## **15. Regulatory Information**

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

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

### **15.2 Chemical Safety Assessment**

<b>Chemical Safety Assessment</b>	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>

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**Other Information**

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**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.