

# SAFETY DATA SHEET

fluorochem.

## 1. Identification of Substance / Mixture

### Product Identifier

1.1.2 Product Name	2-methyl-3,5,6,7,8,9-hexahydro-4H-pyrimido[4,5-d]azepin-4-one dihydrochloride hydrate
1.1.2 Other Names	
1.1.1 Product Code	F360397
1.1.3 CAS	391953-90-5
1.1.4 MDL	MFCD26959516
1.1.5 EINECS	N/A
1.1.6 REACH Registration Number	
1.2.1 Relevant Uses	For research and development purposes only.
1.2.2 Uses Advised Against	No uses advised against.

### 1.3 Supplier Details

1.3.1 Company	Fluorochem Ltd
1.3.2 Address	Unit 14, Graphite Way Hadfield Glossop Derbys. SK13 1QH United Kingdom
1.3.3 Telephone	01457 860111
1.3.4 Email	sds@fluorochem.co.uk
1.4.1 Emergency Telephone	+44 20 3807 3798

## 2. Hazards Identification

### 2.1.1 Classification

Acute Tox. 4  
Eye Irrit. 2A  
Skin Irrit. 2  
STOT SE 3

### 2.2.1 Signal Word

**Warning**

### 2.2.2 Pictograms



GHS07

### 2.2.3 Hazards

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

#### 2.2.4 Precautions

**P261** Avoid breathing dust/fume/gas/mist/vapours/spray.  
**P264** Wash hands thoroughly after handling.  
**P270** Do not eat, drink or smoke when using this product.  
**P271** Use only outdoors or in a well-ventilated area.  
**P280.4** Wear protective gloves/protective clothing and eye/face protection.  
**P301+P330+P331** IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.  
**P303+P361+P353.1** 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.  
**P308+P313** IF exposed or concerned: Get medical advice/attention.  
**P321** Specific treatment.  
**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.  
**P501.3** Dispose of contents/container to hazardous waste disposal.

#### 2.2.5 Other Classification Hazards

### 3. Composition of Ingredients

#### SUBSTANCE

3.1.1 Name	3.1.2 CAS	Einecs	3.1.3 Composition	Hazards
2-methyl-3,5,6,7,8,9-hexahydro-4H-pyrimido[4,5-d]azepin-4-one dihydrochloride hydrate	391953-90-5	N/A		H302 Acute Tox. 4 H315 Skin Irrit. 2 H319 Eye Irrit. 2A H335 STOT SE 3

### 4. First Aid Measures

4.1.1 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.
4.1.2 Ingestion	If swallowed rinse the mouth with plenty of water (only if the person is conscious) and contact a poison centre or physician if you feel unwell.
4.1.3 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.
4.1.4 Skin Contact	Where Diphoterine is not available, wash immediately with plenty of water and soap. Remove contaminated clothing immediately. Immediately seek medical attention.
4.1.5 General Advice	No additional advice.
4.2.1 Most Important Symptoms and Effects	No known symptoms or effects.
4.3.1 Immediate First Aid Measures	No special immediate treatment required

### 5. Fire Fighting Measures

5.1.1 Suitable Fire Extinguishing Media	Carbon dioxide, alcohol resistant foam or dry chemical powder. Use water to extinguish fire.
5.1.2 Unsuitable Fire Extinguishing Media	No known unsuitable media.
5.2.1 Special Hazards	Thermal decomposition can lead to release of irritating gases and vapours.
5.3.1 Advice for Fire Fighters	As in any fire, wear self-contained breathing apparatus and full protective gear.

### 6. Accidental Release Measures

6.1.1 Personal Precautions	Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Keep personnel away from spill/leak.
6.2.1 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.
6.3.1 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.
6.4.1 Referenced SDS Sections	For personal protection see section 8. For disposal see section 13.

### 7. Handling and Storage

#### Personal Precautions

<b>7.1.1 Safe Handling</b>	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.
<b>7.1.2 Protection Against Explosion and Fire</b>	Where possible, use anti static and spark proof equipment when handling.
<b>7.1.3 General Occupational Hygiene</b>	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.

### **Conditions for Safe Storage and Incompatibilities**

<b>7.2.1 Managing Storage Risks</b>	Keep container tightly closed and upright. Store in a cool, dry and well-ventilated place.
<b>7.2.2 Storage Controls</b>	Keep container tightly closed in a cool area away from sunlight or heat sources.
<b>7.2.3 Maintaining Integrity</b>	Keep container tightly closed in a cool area away from sunlight or heat sources.
<b>7.2.4 Other Advice</b>	No other specific advice available.
<b>7.3.1 Specific End Use(s)</b>	No specific end uses are advised. The products supplied are for research purposes only.

## **8. Exposure Controls / Personal Protection**

<b>8.1.1 Control Parameters</b>	
<b>8.2.1 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>8.2.2 Face Protection</b>	Wear tightly fitting safety goggles which adhere to European standard EN 166. Ensure eye bath is to hand.
<b>8.2.3 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>8.2.4 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>8.2.5 Respiratory Protection</b>	Product should be handled in a fume cupboard with adequate extraction. No respiratory equipment is needed under normal use conditions.
<b>8.2.6 Hygiene Protection</b>	Ensure hair or skin particles cannot enter the chemical container.
<b>8.2.7 Environment Exposure Controls</b>	Avoid discharge into the environment, see section 6.2.

## **9. Physical and Chemical Properties**

<b>9.1.1 State</b>	No data available.
<b>9.1.2 Appearance</b>	No data available.
<b>9.1.3 Odour</b>	No data available.
<b>9.1.4 Odour Threshold</b>	No data available.
<b>9.1.5 pH</b>	No data available.
<b>9.1.6 Melting Point / Freezing Point</b>	No data available.
<b>9.1.7 Initial Boiling Point</b>	No data available.
<b>9.1.8 Boiling Range</b>	No data available.
<b>9.1.9 Flash Point</b>	No data available.
<b>9.1.10 Evaporation Rate</b>	No data available.
<b>9.1.11 Flammability</b>	No data available.
<b>9.1.12 Upper / Lower Flammability or Explosion Limits</b>	No data available.
<b>9.1.13 Vapour Pressure</b>	No data available.
<b>9.1.14 Vapour Density</b>	No data available.
<b>9.1.15 Relative Density</b>	No data available.
<b>9.1.16 Solubility</b>	
<b>9.1.17 Partition Coefficient</b>	No data available.
<b>9.1.18 Auto Ignition Temperature</b>	No data available.
<b>9.1.19 Decomposition Temperature</b>	No data available.
<b>9.1.20 Viscosity</b>	No data available.
<b>9.1.21 Explosive Properties</b>	No data available.
<b>9.1.22 Oxidising Properties</b>	No data available.
<b>9.2.1 Other information</b>	No additional information available.

## 10. Stability and Reactivity

10.1.1 Reactivity	No known Reactivity, based on information available.
10.2.1 Stability	Stable under recommended storage conditions.
10.3.1 Possibility of Hazardous Reactions	None under normal storage conditions.
10.4.1 Conditions To Avoid	Heat, sparks, open flames, sources of ignition. Exposure to moisture.
10.5.1 Incompatible Materials	Strong oxidising agents.
10.6.1 Hazardous Decomposition Products	No Data Available.

## 11. Toxicology Information

11.1.1 Acute Toxicity	No Toxicology data available for this product.
11.1.2 Skin Corrosion / Irritation	No Toxicology data available for this product.
11.1.3 Serious Eye Damage / Irritation	No Toxicology data available for this product.
11.1.4 Respiratory or Skin Sensitisation	No Toxicology data available for this product.
11.1.5 Germ Cell Mutagenicity	No Toxicology data available for this product.
11.1.6 Carcinogenicity	No Toxicology data available for this product.
11.1.7 Reproductive Toxicity	No Toxicology data available for this product.
11.1.8 STOT-single Exposure	No Toxicology data available for this product.
11.1.9 STOT-repeated Exposure	No Toxicology data available for this product.
11.1.10 Aspiration Hazard	No Toxicology data available for this product.
11.2.1 Additional Toxicology Information	No Toxicology data available for this product.

## 12. Ecological Information

12.1.1 Toxicity	No Ecological data available for this product.
12.2.1 Persistence and Degradability	No Ecological data available for this product.
12.3.1 Bio-Accumulative Potential	No Ecological data available for this product.
12.4.1 Mobility in Soil	No Ecological data available for this product.
12.5.1 Results of PBT and vPvB assessment	No Ecological data available for this product.
12.7.1 Endocrine Disrupting Properties	Avoid release to the environment.
12.6.1 Other Adverse Effects	No Ecological data available for this product.

## 13. Disposal Considerations

13.1.1 Disposal Operations	Ensure product is disposed of by licensed waste carriers.
13.1.2 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

IATA UN Number	ADR UN Number	IMDG UN Number
14.1.2 IATA Proper Shipping Name (2-methyl-3,5,6,7,8,9-hexahydro-4H-pyrimido [4,5-d]azepin-4-one dihydrochloride hydrate)	ADR Proper Shipping Name Non Hazardous For Transport (2-methyl-3,5,6,7,8,9-hexahydro-4H-pyrimido [4,5-d]azepin-4-one dihydrochloride hydrate)	IMDG Proper Shipping Name (2-methyl-3,5,6,7,8,9-hexahydro-4H-pyrimido [4,5-d]azepin-4-one dihydrochloride hydrate)
IATA Packing Group	ADR Packing Group	IMDG Packing Group
14.1.4 IATA Hazard Class	ADR Hazard Class	IMDG Hazard Class
14.1.5 IATA Sub Class	ADR Sub Class	IMDG Sub Class

## 15. Regulatory Information

15.1.1 Regulatory Information	As far as Fluorochem is aware, there are no further regulations controlling this product.
15.2.1 Chemical Safety Assessment	No Chemical Safety Assessment is available for this product.

## 16. Other Information

**16.1.2 Information Not Covered in Other Sections**

ADR: Accord Europeen sur le transport des marchandises Dangereuses par Route(European Agreement concerning the International Carriage of Dangerous Goods by road)  
RID:Reglement International concernant le transport des marchandises dangereuses par chemin de fer (Regulations concerning the International transport of Dangerous Goods by Rail)  
IMDG: International Maritime Code for Dangerous Goods  
IATA: International Air Transport Association  
IATA-DGR: Dangerous Goods Regulations by the International Air Transport Association ICAO:International Civil Aviation Organization  
ICAO-TI: Technical Instructions by the ICAO  
GHS: Globally Harmonized System of Classification and Labelling of Chemicals  
CAS:Chemical Abstracts Service

**Revision**

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**Date Modified**

Oct 11, 2023 1:54:00 PM

**16.1.1 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 physicochemical 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 information 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.