

# SAFETY DATA SHEET

fluorochem.

## 1. Identification of Substance / Mixture

### Product Identifier

1.1.2 Product Name	2-Butyl-3-[2'-(1H-tetrazol-5-yl)biphenyl-4-ylmethyl]1,3-diaza-spiro[4.4]non-1-en-4-one
1.1.2 Other Names	
1.1.1 Product Code	F036499
1.1.3 CAS	138402-11-6
1.1.4 MDL	MFCD00864464
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

Eye Irrit. 2A  
Skin Irrit. 2  
STOT SE 3

### 2.2.1 Signal Word

**Warning**

### 2.2.2 Pictograms



GHS07

### 2.2.3 Hazards

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.  
P271 Use only outdoors or in a well-ventilated area.  
P280.4 Wear protective gloves/protective clothing and eye/face protection.  
P302+P352.2 IF ON SKIN: Wash with plenty of water and soap.  
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.  
P312.1 Call a POISON CENTER/doctor if you feel unwell.  
P321 Specific treatment.  
P332+P313 If skin irritation occurs: Get medical advice/attention.  
P337+P313 If eye irritation persists: Get medical advice/attention.  
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.

## 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-Butyl-3-[2'-(1H-tetrazol-5-yl)biphenyl-4-ylmethyl]1,3-diazaspiro[4.4]non-1-en-4-one	138402-11-6	N/A		H315 Skin Irrit. 2 H319 Eye Irrit. 2A H335 STOT SE 3

## 4. First Aid Measures

4.1.1 Eye contact	In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart. Protect uninjured eye. Remove contact lenses, if present and easy to do. Continue rinsing and seek medical attention.
4.1.2 Ingestion	Where Diphoterine is not available, rinse mouth with copious amounts of water. Seek urgent medical advice.
4.1.3 Inhalation	Remove person to fresh air and keep comfortable for breathing. If experiencing respiratory problems seek immediate medical attention.
4.1.4 Skin Contact	After contact with skin, wash immediately with plenty of water and soap. Remove contaminated clothing immediately. In case of skin reactions, consult a physician.
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. Ensure Hexafluorine washing solution is to hand. 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	

## 7. Handling and Storage

*Personal Precautions*

7.1.1 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.
7.1.2 Protection Against Explosion and Fire	Where possible, use anti static and spark proof equipment when handling.
7.1.3 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.

*Conditions for Safe Storage and Incompatibilities*

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

## 8. Exposure Controls / Personal Protection

### 8.1.1 Control Parameters

<b>8.2.1 Engineering Measures</b>	Use only under a chemical fume hood ensuring adequate ventilation, especially in confined areas. Ensure Hexafluorine washing solution is close to workstation. 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 Hexafluorine eye wash 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. Ensure Hexafluorine washing solution is to hand. 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>	Solid
<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>	Dimethyl sulfoxide(DMSO)
<b>9.1.17 Partition Coefficient</b>	4
<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

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

## 11. Toxicology Information

<b>11.1.1 Acute Toxicity</b>	No Toxicology data available for this product.
<b>11.1.2 Skin Corrosion / Irritation</b>	No Toxicology data available for this product.
<b>11.1.3 Serious Eye Damage / Irritation</b>	No Toxicology data available for this product.
<b>11.1.4 Respiratory or Skin Sensitisation</b>	No Toxicology data available for this product.

<b>11.1.5 Germ Cell Mutagenicity</b>	No Toxicology data available for this product.
<b>11.1.6 Carcinogenicity</b>	No Toxicology data available for this product.
<b>11.1.7 Reproductive Toxicity</b>	No Toxicology data available for this product.
<b>11.1.8 STOT-single Exposure</b>	No Toxicology data available for this product.
<b>11.1.9 STOT-repeated Exposure</b>	No Toxicology data available for this product.
<b>11.1.10 Aspiration Hazard</b>	No Toxicology data available for this product.
<b>11.2.1 Additional Toxicology Information</b>	No Toxicology data available for this product.

## 12. Ecological Information

<b>12.1.1 Toxicity</b>	No Ecological data available for this product.
<b>12.2.1 Persistence and Degradability</b>	No Ecological data available for this product.
<b>12.3.1 Bio-Accumulative Potential</b>	No Ecological data available for this product.
<b>12.4.1 Mobility in Soil</b>	Log Pow: 4
<b>12.5.1 Results of PBT and vPvB assessment</b>	No Ecological data available for this product.
<b>12.7.1 Endocrine Disrupting Properties</b>	No Ecological data available for this product.
<b>12.6.1 Other Adverse Effects</b>	No Ecological data available for this product.

## 13. Disposal Considerations

<b>13.1.1 Disposal Operations</b>	Ensure product is disposed of by licensed waste carriers.
<b>13.1.2 Disposal of Packaging</b>	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
<b>14.1.2 IATA Proper Shipping Name</b>	<b>ADR Proper Shipping Name</b>	<b>IMDG Proper Shipping Name</b>
(2-Butyl-3-[2'-(1H-tetrazol-5-yl)biphenyl-4-ylmethyl]1,3-diaza-spiro[4.4]non-1-en-4-one)	Non Hazardous For Transport (2-Butyl-3-[2'-(1H-tetrazol-5-yl)biphenyl-4-ylmethyl]1,3-diaza-spiro[4.4]non-1-en-4-one)	(2-Butyl-3-[2'-(1H-tetrazol-5-yl)biphenyl-4-ylmethyl]1,3-diaza-spiro[4.4]non-1-en-4-one)
<b>IATA Packing Group</b>	<b>ADR Packing Group</b>	<b>IMDG Packing Group</b>
<b>14.1.4 IATA Hazard Class</b>	<b>ADR Hazard Class</b>	<b>IMDG Hazard Class</b>
<b>14.1.5 IATA Sub Class</b>	<b>ADR Sub Class</b>	<b>IMDG Sub Class</b>

## 15. Regulatory Information

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

## 16. Other Information

<b>16.1.2 Information Not Covered in Other Sections</b>	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
<b>Revision</b>	1
<b>Date Modified</b>	Aug 10, 2023 12:34:00 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.