

Safety Data Sheet

fluorochem.

1. Identification of the substance/mixture

1.1 Product identification

Product name	3-[(4-nitro-1H-pyrazol-1-yl)methyl]benzonitrile
Other names	
Product code	F524926
CAS	957501-01-8
MDL	MFCD02029353
EINECS	N/A
REACH Registration number	

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

Signal Word

Warning

Pictograms



GHS07

Hazards

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

Precautions

P101 If medical advice is needed, have product container or label at hand.
P264 Wash hands thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P362+P364 Take off contaminated clothing and wash it before reuse.
P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P302+P352 IF ON SKIN: Wash with plenty of water and soap.
P405 Store locked up.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/protective clothing and eye/face protection.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.
P308+P313 IF exposed or concerned: Get medical advice/attention.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P321 Specific treatment (see Section 4 on this SDS).
P501 Dispose of contents/container to hazardous waste disposal.

2.3 Other Hazards

Other Classification Hazards

3. Composition

3.1 SUBSTANCE

Name	CAS	Einecs	Composition	Hazards
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3-[(4-nitro-1H-
pyrazol-1-
yl)methyl]benzonitrile

957501-01-8

N/A

3.2 MIXTURE

Not applicable. Product is a substance.

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	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.
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	No additional advice.

4.2 Most Important Symptoms and Effects

Most Important Symptoms and Effects No known symptoms or effects.

4.3 Indication of any urgent medical attention and special treatments needed

Immediate First Aid Measures No special immediate treatment required.

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.

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.

8. Exposure Controls / Personal Protection

8.1 Control Parameters

Control Parameters

No data available.

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.

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.
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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

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

Incompatible Materials	Strong oxidizing agents.
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10.6 Hazardous Decomposition Products

Hazardous Decomposition Products	No data available.
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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

Endocrine Disrupting Properties	Avoid release to the environment.
Addition Toxicology Information	No Toxicology data available for this product.

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

Endocrine Disrupting Properties	Avoid release to the environment.
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12.7 Other Adverse Effects

Other Adverse Effects	Avoid release to the environment.
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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	(3-[(4-nitro-1H-pyrazol-1-yl)methyl]benzo nitrile)	ADR Proper Shipping Name	Non Hazardous For Transport (3-[(4-nitro-1H-pyrazol-1-yl)methyl]benzo nitrile)	IMDG Proper Shipping Name	(3-[(4-nitro-1H-pyrazol-1-yl)methyl]benzo nitrile)
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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 Enviromental 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	As far as Fluorochem is aware, there are no further regulations controlling this product.
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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

ional transport of dangerous goods by road). RID: International Regulations concerning the Transport of Dangerous Goods by Rail (Regulations regarding 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 fra International Air Transport Association. ICAO: International Civil Aviation Organisation. ICAO-TI: Technical instructions from ICAO. GHS: Globally Harmonized System for Classification and Labelling of Chemicals. CAS: Chemical Abstracts Service

Other Information

Revision	1
Date Modified	19/12/2024 18:46:00
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 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.