

SAFETY DATA SHEET

1. PRODUCT AND COMPANY IDENTIFICATION**1.1 Product identifier**

Reference: DA003NXT

CAS number: 446-86-6

Name: 6-((1-Methyl-4-nitro-1H-imidazol-5-yl)thio)-9H-purine

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

Identified uses: Laboratory chemicals. manufacture of chemical compounds

Restrictions on use: For use in laboratory only.

1.3 Supplier

Company: Indagoo Research Chemicals

Registry number: 81777290

REACH number. No data available

2. HAZARDS IDENTIFICATION**2.1 Classification of the substance or mixture under CLP according to (EC) 1272/2008**

Acute toxicity. oral.(Category 4). H302

Skin corrosion/irritation.(Category 2). H315

Serious eye damage/eye irritation.(Category 2A). H319

Specific target organ toxicity. single exposure; Respiratory tract irritation.(Category 3). H335

Carcinogenicity.(Category 1A. 1B). H350

Reproductive toxicity.(Category 1A. 1B). H360

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

2.2 Label elements

Signal word: warning

Hazard statements

H302 Harmful if swallowed

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

H350 May cause cancer

H360 May damage fertility or the unborn child

Precautionary statements

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes.Remove contactlenses.if present and easy to do. Continue rinsing.

2.3 Other hazards

None

3. COMPOSITION/INFORMATION ON INGREDIENTS

Chemical Name: 6-((1-Methyl-4-nitro-1H-imidazol-5-yl)thio)-9H-purine

CAS Number: 446-86-6

Molecular Formula: C₉H₇N₇O₂S

Molecular Weight: 277.2626 g/mol

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2 or section 11)

4.3 Indication of any immediate medical attention and special treatment needed

no data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides, nitrogen oxides (NO_x), Hydrogen bromide gas

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.
Provide appropriate exhaust ventilation at places where dust is formed.
Normal measures for preventive fire protection.
For precautions see section 2.

7.2 Conditions for safe storage, including any incompatibilities

Keep in dry area.
-10 °C.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1. no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. 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.

Body protection

Complete suit protecting against chemicals. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Appearance / Physical state: solid

Odour: no data available

Odour threshold: no data available
pH: no data available
Melting point: 243-244°C
Boiling point: 555.8°C at 760 mmHg
Flash point: no data available
Evaporation rate: no data available
Flammability: no data available
Upper/lower flammability or explosive limits: No data available
Vapour pressure: no data available
Vapour density: no data available
Relative density: no data available
Water solubility: no data available
Partition coefficient (n-octanol/water): no data available
Auto-ignition temperature: no data available
Decomposition temperature: no data available
Log Pow: no data available
Viscosity: no data available
Explosive properties: no data available
Oxidising properties: no data available

9.2. Other safety information

no data available

10. STABILITY AND REACTIVITY

- 10.1 **Reactivity:** no data available
10.2 **Chemical stability:** Stable under recommended storage conditions.
10.3 **Possibility of hazardous reactions:** no data available
10.4 **Conditions to avoid:** no data available
10.5 **Incompatible materials:** no data available
10.6 **Hazardous decomposition products:** no data available
10.7 **In case of fire:** See section 5

11. TOXICOLOGICAL INFORMATION

- 11.1 **Acute toxicity:** Classified based on available data. For more details, see section 2
11.2 **Skin corrosion:** Classified based on available data. For more details, see section 2
11.3 **Serious eye damage:** Classified based on available data. For more details, see section 2
11.4 **Respiratory or skin sensitisation:** Classified based on available data. For more details, see section 2
11.5 **Germ cell mutagenicity:** Classified based on available data. For more details, see section 2
11.6 **Carcinogenicity:**
 11.6.1 **IARC:** No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC
 11.6.2 **ACGIH:** No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH
 11.6.3 **NTP:** No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP
 11.6.4 **OSHA:** No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
11.7 **Reproductive toxicity**
 11.7.1. **Specific target organ toxicity – single exposure:** no data available
 11.7.2. **Specific target organ toxicity – repeated exposure:** no data available

11.8 Aspiration hazard: no data available

11.9 Additional information: no data available

12. ECOLOGICAL INFORMATION

12.1 Toxicity: no data available

12.2 Persistence and degradability: no data available

12.3 Bioaccumulative potential: no data available

12.4 Mobility in soil: no data available

12.5 Results of PBT and vPvB assessment: PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties: No data available

12.7 Other adverse effects: no data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste from residues / unused products: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

13.2 Contaminated packaging: Dispose of as unused product.

13.3 European Waste Catalogue (EWC): No data available

14. TRANSPORT INFORMATION

14.1 UN number

ADR/RID: IMDG: IATA-DGR:

14.2 Proper shipping name

ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA-DGR: Not dangerous goods

14.3 Transport hazard class(es)

ADR/RID: IMDG: IATA-DGR:

14.4 Packing group

ADR/RID: IMDG: IATA-DGR:

14.5 Environmental hazards

ADR/RID: - IMDG: - IATA-DGR: -

14.6 Special precautions for user

No data available

14.7 Transport in bulk according to IMO instruments

No data available

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

Component:

6-((1-Methyl-4-nitro-1H-imidazol-5-yl)thio)-9H-purine

Regulation:

REACH (1907/2006) - Annex XIV - Substances subject to authorization

REACH (1907/2006) - Annex XVII - Restrictions on certain hazardous substances

REACH Regulation (EC 1907/2006) Article 59 - Candidate List of Substances of Very High Concern (SVHC)

Regulatory listings:

EINECS, IECSC, ENCS, TCSI, TSCA, NZIOC, PICCS, AICS, DSL

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out.

16. OTHER INFORMATION**Full text of H-Statements referred to under sections 2 and 3.**

H302 Harmful if swallowed

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

H350 May cause cancer

H360 May damage fertility or the unborn child

Abbreviations Full Texts

ADN European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways

ADR European Agreement concerning the International Carriage of Dangerous Goods by Road

ALARP As low as is reasonably practicable

CAS Chemical Abstracts Service

CLP Classification, Labelling and Packaging Regulations

COSHH Control of Substances Hazardous to Health

EC Number European Community Number

EC50 Effective Concentration 50%

EILINCS European List of Notified Chemical Substances

EINECS European Inventory of Existing Commercial Chemical Substances

GHS Globally Harmonised System

HSE Health & Safety Executive UK

IATA International Air Transport Association

IM Intramuscular

IMDG The International Maritime Dangerous Goods Code

IP Intraperitoneal

IV Intravascular

LD50 Lethal Dose 50%

LOEC Lowest Observable Effective Concentration

LTEL Long Term Exposure Limit

NOEC No Observable Effective Concentration

OECD Organisation for Economic Cooperations and Development

PBT Persistent Bioaccumulative Toxic

PPE Personal Protective Equipment

REACH Registration, Evaluation, Authorisation and Restriction of Chemicals

RID Regulations Concerning the International Carriage of Dangerous Goods by Rail

SC Subcutaneous

SDS Safety Data Sheet

STEL Short Term Exposure Limit

STOT Specific Target Organ Toxicity

VOC Volatile Organic Compounds

vPvB Very Persistent and Very Bioaccumulative

WEL Workplace Exposure Limits

Training advice:

Training on chemical hazard awareness, including labeling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE), and hygiene

Further information

The above information is believed to be correct but does not purport to be exhaustive and should be used only as a guide. The information in this document is based on our current knowledge and is applicable to the product only with regard to appropriate safety precautions. It does not constitute a guarantee of the product's properties.

Disclaimer: Indagoo Research Chemicals shall not be held liable for any damage resulting from handling or contact with the above product. The information provided is believed to be accurate but is not intended to be all-inclusive and shall be used only as a guide. This document does not guarantee the properties or quality of the product.

This Safety Data Sheet has been prepared in accordance with Commission Regulation (EC) No. 1907/2006, as amended by Commission Regulation (EU) 2020/878.