



SAFETY DATA SHEET

6-Mercaptopurine monohydrate

According to the REACH etc. (Amendment etc.) (EU Exit) Regulations 2020 No. 1577, as amended.

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product name	6-Mercaptopurine monohydrate
CAS number	6112-76-1
EC number	200-037-4

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

Identified uses	Research and development.
Uses advised against	Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier	Molekula Ltd. Lingfield Way, Darlington, DL1 4XX, United Kingdom +44 (0) 3302000333 info@molekula.com
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1.4. Emergency telephone number

+44 (0) 7769276927

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (SI 2019 No. 720)

Physical hazards	Not Classified
Health hazards	Acute Tox. 3 - H301 Skin Irrit. 2 - H315 Eye Irrit. 2 - H319 Muta. 1B - H340 Carc. 2 - H351 Repr. 1B - H360 STOT RE 1 - H372
Environmental hazards	Not Classified

2.2. Label elements

EC number	200-037-4
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Hazard pictograms



Signal word	Danger
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Hazard statements	H301 Toxic if swallowed. H315 Causes skin irritation. H319 Causes serious eye irritation. H340 May cause genetic defects. H351 Suspected of causing cancer. H360 May damage fertility or the unborn child. H372 Causes damage to organs (Bone marrow, Liver) through prolonged or repeated exposure.
Precautionary statements	P201 Obtain special instructions before use. P202 Do not handle until all safety precautions have been read and understood. P260 Do not breathe dust. P264 Wash contaminated skin thoroughly after handling. P270 Do not eat, drink or smoke when using this product. P280 Wear protective gloves/ protective clothing/ eye protection/ face protection. P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. P302+P352 IF ON SKIN: Wash with plenty of water. 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. P330 Rinse mouth. 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. P405 Store locked up. P501 Dispose of contents/ container in accordance with national regulations.

2.3. Other hazards

This substance is not classified as PBT or vPvB according to current UK criteria.

SECTION 3: Composition/information on ingredients

3.1. Substances

Product name	6-Mercaptopurine monohydrate
CAS number	6112-76-1
EC number	200-037-4
Chemical formula	C ₅ H ₄ N ₄ S · H ₂ O

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	Get medical attention if any discomfort continues. Show this Safety Data Sheet to the medical personnel.
Inhalation	Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Loosen tight clothing such as collar, tie or belt. Get medical attention if symptoms are severe or persist.
Ingestion	If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.
Skin contact	Rinse with water.

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Eye contact Rinse with water. Do not rub eye. Remove any contact lenses and open eyelids wide apart. Get medical attention if any discomfort continues.

Protection of first aiders It may be dangerous for first aid personnel to carry out mouth-to-mouth resuscitation.

4.2. Most important symptoms and effects, both acute and delayed

General information The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation Prolonged or repeated exposure may cause the following adverse effects: Suspected of causing cancer.

Ingestion May cause stomach pain or vomiting. May cause severe internal injury. Prolonged or repeated exposure may cause the following adverse effects: Suspected of causing cancer.

Skin contact Redness. Irritating to skin. Prolonged or repeated exposure may cause the following adverse effects: Suspected of causing cancer.

Eye contact Irritating to eyes.

4.3. Indication of any immediate medical attention and special treatment needed

Notes for the doctor Treat symptomatically. Keep affected person under observation.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.

Unsuitable extinguishing media Do not use water jet as an extinguisher, as this will spread the fire.

5.2. Special hazards arising from the substance or mixture

Specific hazards This product is toxic.

Hazardous combustion products Thermal decomposition or combustion products may include the following substances: Very toxic or corrosive gases or vapours.

5.3. Advice for firefighters

Protective actions during firefighting Avoid breathing fire gases or vapours. Evacuate area. Keep upwind to avoid inhalation of gases, vapours, fumes and smoke. Ventilate closed spaces before entering them. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. Control run-off water by containing and keeping it out of sewers and watercourses. If risk of water pollution occurs, notify appropriate authorities.

Special protective equipment for firefighters Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing will provide a basic level of protection for chemical incidents.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material.

6.2. Environmental precautions

Environmental precautions Avoid discharge into drains or watercourses or onto the ground. Avoid discharge to the aquatic environment.

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6.3. Methods and material for containment and cleaning up

Methods for cleaning up	Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. Provide adequate ventilation. Collect spillage with a shovel and broom, or similar and reuse, if possible. Collect and place in suitable waste disposal containers and seal securely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. For waste disposal, see Section 13.
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6.4. Reference to other sections

Reference to other sections	For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.
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SECTION 7: Handling and storage

7.1. Precautions for safe handling

Usage precautions	Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Keep container tightly sealed when not in use. This product is toxic. Immediate first aid is imperative. Suspected of causing cancer. May cause genetic defects. May damage fertility or the unborn child. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. Do not reuse empty containers.
Advice on general occupational hygiene	Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions	Store away from incompatible materials (see Section 10). Store locked up. Keep only in the original container. Keep container tightly closed, in a cool, well ventilated place. Keep containers upright. Protect containers from damage.
Storage class	Combustible, acutely toxic Cat. 3 / toxic or chronic hazardous substances

7.3. Specific end use(s)

Specific end use(s)	The identified uses for this product are detailed in Section 1.2.
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SECTION 8: Exposure controls/Personal protection

8.1. Control parameters

Occupational exposure limits

STEL:

TWA:

8.2. Exposure controls

Protective equipment



Appropriate engineering controls

Provide adequate general and local exhaust ventilation. Ensure the ventilation system is regularly maintained and tested. Good general ventilation should be adequate to control worker exposure to airborne contaminants. Observe any occupational exposure limits for the product or ingredients.

Eye/face protection

Wear tight-fitting, chemical splash goggles or face shield. If inhalation hazards exist, a full-face respirator may be required instead.

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Hand protection	Wear protective gloves. The most suitable glove should be chosen in consultation with the glove supplier/manufacture, who can provide information about the breakthrough time of the glove material. To protect hands from chemicals, wear gloves that are proven to be impervious to the chemical and resist degradation. Considering the data specified by the glove manufacturer, check during use that the gloves are retaining their protective properties and change them as soon as any deterioration is detected. Frequent changes are recommended.
Other skin and body protection	Wear appropriate clothing to prevent any possibility of skin contact.
Hygiene measures	Wash after use and before eating, smoking and using the toilet. Do not eat, drink or smoke when using this product.
Respiratory protection	Ensure all respiratory protective equipment is suitable for its intended use and is 'UKCA'-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges suitable for intended use should be used. Full face mask respirators with replaceable filter cartridges suitable for intended use should be used. Half mask and quarter mask respirators with replaceable filter cartridges suitable for intended use should be used.
Environmental exposure controls	Keep container tightly sealed when not in use. Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	Powder.
Colour	Yellow-white.
Odour	Odourless.
Odour threshold	No information available.
pH	No information available.
Melting point	~ 313°C/595.4°F
Initial boiling point and range	No information available.
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Upper/lower flammability or explosive limits	No information available.
Vapour pressure	No information available.
Vapour density	No information available.
Relative density	No information available.
Solubility(ies)	No information available.
Partition coefficient	No information available.
Auto-ignition temperature	No information available.
Decomposition Temperature	No information available.

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9.2. Other information

Molecular weight 170.19

SECTION 10: Stability and reactivity

10.1. Reactivity

Reactivity This is a combustible organic substance. The risk of a dust explosion may be assumed when the substance is finely distributed.

10.2. Chemical stability

Stability Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Possibility of hazardous reactions Violent reactions possible with:
Strong oxidising agents.
Strong acids.
Strong alkalis.

10.4. Conditions to avoid

Conditions to avoid There are no known conditions that are likely to result in a hazardous situation.

10.5. Incompatible materials

Materials to avoid No specific material or group of materials is likely to react with the product to produce a hazardous situation.

10.6. Hazardous decomposition products

Hazardous decomposition products Does not decompose when used and stored as recommended. Thermal decomposition or combustion products may include the following substances: Toxic gases or vapours. Carbon dioxide (CO₂). Carbon monoxide (CO). Sulphurous gases (SO_x).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

Summary Toxic if swallowed.

Acute toxicity oral (LD₅₀ mg/kg) 277.0

Species Rat

ATE oral (mg/kg) 277.0

Acute toxicity - dermal

Summary Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Summary Based on available data the classification criteria are not met.

Skin corrosion/irritation

Summary Causes skin irritation.

Serious eye damage/irritation

Summary Causes serious eye irritation.

Respiratory sensitisation

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Summary	Based on available data the classification criteria are not met.
<u>Skin sensitisation</u>	
Summary	Based on available data the classification criteria are not met.
<u>Germ cell mutagenicity</u>	
Summary	May cause genetic defects.
<u>Carcinogenicity</u>	
Summary	Suspected of causing cancer.
IARC carcinogenicity	None of the ingredients are listed or exempt.
<u>Reproductive toxicity</u>	
Summary	May damage fertility or the unborn child.
<u>Specific target organ toxicity - single exposure</u>	
Summary	Based on available data the classification criteria are not met.
<u>Specific target organ toxicity - repeated exposure</u>	
Summary	Causes damage to organs through prolonged or repeated exposure.
<u>Aspiration hazard</u>	
Summary	Not relevant. Solid.
General information	May damage fertility. May cause cancer after repeated exposure. Risk of cancer depends on duration and level of exposure. May cause genetic defects. The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Temporary irritation.
Ingestion	May cause stomach pain or vomiting. May cause severe internal injury.
Skin contact	Redness. Irritating to skin.
Eye contact	Irritating to eyes.
Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	No specific target organs known.

SECTION 12: Ecological information

Ecotoxicity	Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.
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12.1. Toxicity

Acute aquatic toxicity

Summary	Based on available data the classification criteria are not met.
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Chronic aquatic toxicity

Summary	Based on available data the classification criteria are not met.
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12.2. Persistence and degradability

Persistence and degradability	The degradability of the product is not known.
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12.3. Bioaccumulative potential

Bioaccumulative potential	No data available on bioaccumulation.
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Partition coefficient	No information available.
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12.4. Mobility in soil

Mobility No data available.

12.5. Results of PBT and vPvB assessment

12.6. Other adverse effects

Other adverse effects None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

General information The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered. Care should be taken when handling emptied containers that have not been thoroughly cleaned or rinsed out. Empty containers or liners may retain some product residues and hence be potentially hazardous.

Disposal methods Do not empty into drains. Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste, residues, empty containers, discarded work clothes and contaminated cleaning materials should be collected in designated containers, labelled with their contents. Incineration or landfill should only be considered when recycling is not feasible.

SECTION 14: Transport information

General For limited quantity packaging/limited load information, consult the relevant modal documentation using the data shown in this section.

14.1. UN number

UN No. (ADR/RID)	2811
UN No. (IMDG)	2811
UN No. (ICAO)	2811
UN No. (ADN)	2811

14.2. UN proper shipping name

Proper shipping name (ADR/RID)	TOXIC SOLID, ORGANIC, N.O.S. (6-Mercaptopurine monohydrate)
Proper shipping name (IMDG)	TOXIC SOLID, ORGANIC, N.O.S. (6-Mercaptopurine monohydrate)
Proper shipping name (ICAO)	TOXIC SOLID, ORGANIC, N.O.S. (6-Mercaptopurine monohydrate)
Proper shipping name (ADN)	TOXIC SOLID, ORGANIC, N.O.S. (6-Mercaptopurine monohydrate)

14.3. Transport hazard class(es)

ADR/RID class	6.1
ADR/RID classification code	T2
ADR/RID label	6.1
IMDG class	6.1
ICAO class/division	6.1
ADN class	6.1

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Transport labels



14.4. Packing group

ADR/RID packing group	III
IMDG packing group	III
ICAO packing group	III
ADN packing group	III

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant

No.

14.6. Special precautions for user

Always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

EmS	F-A, S-A
ADR transport category	2
Emergency Action Code	2X
Hazard Identification Number (ADR/RID)	60
Tunnel restriction code	(E)

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Not applicable.

Annex II of MARPOL 73/78
and the IBC Code

SECTION 15: Regulatory information

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

National regulations	Health and Safety at Work etc. Act 1974 (as amended). The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"]. EH40/2005 Workplace exposure limits.
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15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

Inventories

EU - EINECS/ELINCS

None of the ingredients are listed or exempt.

SECTION 16: Other information

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Abbreviations and acronyms used in the safety data sheet	ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.
	ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.
	RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.
	IATA: International Air Transport Association.
	ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air.
	IMDG: International Maritime Dangerous Goods.
	CAS: Chemical Abstracts Service.
	ATE: Acute Toxicity Estimate.
	LC50: Lethal Concentration to 50 % of a test population.
	LD50: Lethal Dose to 50% of a test population (Median Lethal Dose).
	EC ₅₀ : 50% of maximal Effective Concentration.
	PBT: Persistent, Bioaccumulative and Toxic substance.
	vPvB: Very Persistent and Very Bioaccumulative.
Classification abbreviations and acronyms	Acute Tox. = Acute toxicity
	Carc. = Carcinogenicity
	Eye Irrit. = Eye irritation
	Muta. = Germ cell mutagenicity
	Repr. = Reproductive toxicity
	Skin Irrit. = Skin irritation
Classification procedures according to SI 2019 No. 720	STOT RE = Specific target organ toxicity-repeated exposure
Training advice	Acute Tox. 3 - H301: STOT RE 1 - H372: Skin Irrit. 2 - H315: Eye Irrit. 2 - H319: Muta. 1B - H340: Carc. 2 - H351: Repr. 1B - H360: : Expert judgement.
	Only trained personnel should use this material.
Revision date	23/05/2023
Revision	1
SDS number	2300
Hazard statements in full	H301 Toxic if swallowed.
	H315 Causes skin irritation.
	H319 Causes serious eye irritation.
	H340 May cause genetic defects.
	H351 Suspected of causing cancer.
	H360 May damage fertility or the unborn child.
	H372 Causes damage to organs (Bone marrow, Liver) through prolonged or repeated exposure.

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.