SAFETY DATA SHEET

1,5,7-Triazabicyclo(4.4.0)dec-5-ene (1,3,4,6,7,8-hexahydro-2H-pyrimido(1,2-a)pyrimidine)

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 1,5,7-Triazabicyclo(4.4.0)dec-5-ene (1,3,4,6,7,8-hexahydro-2H-pyrimido(1,2-a)pyrimidine)

Product number 18977285

CAS number 5807-14-7

EC number 227-367-1

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

Identified uses For research purposes only.

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

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 Skin Corr. 1B - H314 Eye Dam. 1 - H318

Environmental hazards Not Classified

2.2. Label elements

EC number 227-367-1

Hazard pictograms



Signal word Danger

Hazard statements H314 Causes severe skin burns and eye damage.

1,5,7-Triazabicyclo(4.4.0)dec-5-ene (1,3,4,6,7,8-hexahydro-2H-pyrimido(1,2-a)pyrimidine)

Precautionary statements

P260 Do not breathe dust.
P264 Wash contaminated skin thoroughly after handling.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
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.
P310 Immediately call a POISON CENTER/ doctor.
P363 Wash contaminated clothing 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	1,5,7-Triazabicyclo(4.4.0)dec-5-ene (1,3,4,6,7,8-hexahydro-2H-pyrimido(1,2-a)pyrimidine)
CAS number	5807-14-7
EC number	227-367-1
Chemical formula	C7H13N3

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. Chemical burns must be treated by a physician.

Inhalation

Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Maintain an open airway. Loosen tight clothing such as collar, tie or belt. Rinse nose and mouth with water. Never give anything by mouth to an unconscious person. Get medical attention if symptoms are severe or persist.

Ingestion

Rinse mouth thoroughly with water. Give a few small glasses of water or milk to drink. Stop if the affected person feels sick as vomiting may be dangerous. Get medical attention.

Skin contact

It is important to remove the substance from the skin immediately. Rinse immediately with plenty of water. Continue to rinse for at least 15 minutes and get medical attention. Chemical burns must be treated by a physician.

Eye contact

Rinse immediately with plenty of water. Do not rub eye. Remove any contact lenses and open eyelids wide apart. Continue to rinse for at least 15 minutes and get medical attention.

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

A single exposure may cause the following adverse effects: Severe irritation of nose and throat. Symptoms following overexposure may include the following: Corrosive to the respiratory tract.

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Ingestion	May cause chemical burns in mouth, oesophagus and stomach. Symptoms following overexposure may include the following: Severe stomach pain. Nausea, vomiting.
Skin contact	Causes severe burns. Symptoms following overexposure may include the following: Pain or irritation. Redness. Blistering may occur.
Eye contact	Causes serious eye damage. Symptoms following overexposure may include the following: Pain. Profuse watering of the eyes. Redness.

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

Notes for the doctor	Treat symptomatically.

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	Severe corrosive hazard. Water used for fire extinguishing, which has been in contact with the product, may be corrosive.
Hazardous combustion products	Thermal decomposition or combustion products may include the following substances: Very toxic or corrosive gases or vapours. Carbon dioxide (CO_2). Carbon monoxide (CO). Oxides of nitrogen.

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. 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. Avoid discharge to the aquatic environment. 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	Regular protection may not be safe. Wear chemical protective suit. 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. Avoid inhalation of dust. Use suitable respiratory protection if ventilation is inadequate. Avoid contact with skin and eyes.

6.2. Environmental precautions

Environmental precautions	The product may affect the acidity (pH) of water which may have hazardous effects on aquatic organisms. Avoid discharge to the aquatic environment.

6.3. Methods and material for containment and cleaning up

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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. This product is corrosive. 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.

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.

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 corrosive. Immediate first aid is imperative. 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 Corrosive storage.

7.3. Specific end use(s)

Specific end use(s) The identified uses for this product are detailed in Section 1.2.

SECTION 8: Exposure controls/Personal protection

8.1. Control parameters

8.2. Exposure controls

Protective equipment



Appropriate engineering controls Provide adequate ventilation. 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.

Hand protection Wear protective gloves. The most suitable glove should be chosen in consultation with the glove supplier/manufacturer, 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.

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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	Solid.
Colour	White. to Light (or pale). Yellow.
Odour	Not known.
Odour threshold	No information available.
pH	No information available.
Melting point	125-130°C/257-266°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.

9.2. Other information

Molecular weight	139.20

SECTION 10: Stability and reactivity

10.1. Reactivity

1,5,7-Triazabicyclo(4.4.0)dec-5-ene (1,3,4,6,7,8-hexahydro-2H-pyrimido(1,2-a)pyrimidine)

Reactivity	See the other subsections of this section for further details.

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	No potentially hazardous reactions known.

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	Carbon dioxide (CO_2).

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: Corrosive gases or vapours. Carbon dioxide (CO_2). Carbon monoxide (CO). Oxides of nitrogen.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

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

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 severe skin burns and eye damage.

Serious eye damage/irritation

Summary	Causes serious eye damage.

Respiratory sensitisation

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

Skin sensitisation

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

Germ cell mutagenicity

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

Carcinogenicity

Summary	Based on available data the classification criteria are not met.
IARC carcinogenicity	None of the ingredients are listed or exempt.

Reproductive toxicity

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

Specific target organ toxicity - single exposure

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

Specific target organ toxicity - repeated exposure

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

Aspiration hazard

Summary Not relevant. Solid.

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

Inhalation Corrosive to the respiratory tract. Symptoms following overexposure may include the following: Severe irritation of nose and throat.

Ingestion May cause chemical burns in mouth, oesophagus and stomach. Symptoms following overexposure may include the following: Severe stomach pain. Nausea, vomiting.

Skin contact Causes severe burns. Symptoms following overexposure may include the following: Pain or irritation. Redness. Blistering may occur.

Eye contact Causes serious eye damage. Symptoms following overexposure may include the following: Pain. Profuse watering of the eyes. Redness.

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.

12.1. Toxicity

Acute aquatic toxicity

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

Chronic aquatic toxicity

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

12.2. Persistence and degradability

Persistence and degradability The degradability of the product is not known.

12.3. Bioaccumulative potential

Bioaccumulative potential No data available on bioaccumulation.

Partition coefficient No information available.

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

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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) 1759

UN No. (IMDG) 1759

UN No. (ICAO) 1759

UN No. (ADN) 1759

14.2. UN proper shipping name

Proper shipping name (ADR/RID) CORROSIVE SOLID, N.O.S. (1,5,7-Triazabicyclo(4.4.0)dec-5-ene (1,3,4,6,7,8-hexahydro-2H-pyrimido(1,2-a)pyrimidine))

Proper shipping name (IMDG) CORROSIVE SOLID, N.O.S. (1,5,7-Triazabicyclo(4.4.0)dec-5-ene (1,3,4,6,7,8-hexahydro-2H-pyrimido(1,2-a)pyrimidine))

Proper shipping name (ICAO) CORROSIVE SOLID, N.O.S. (1,5,7-Triazabicyclo(4.4.0)dec-5-ene (1,3,4,6,7,8-hexahydro-2H-pyrimido(1,2-a)pyrimidine))

Proper shipping name (ADN) CORROSIVE SOLID, N.O.S. (1,5,7-Triazabicyclo(4.4.0)dec-5-ene (1,3,4,6,7,8-hexahydro-2H-pyrimido(1,2-a)pyrimidine))

14.3. Transport hazard class(es)

ADR/RID class 8

ADR/RID classification code C10

ADR/RID label 8

IMDG class 8

ICAO class/division 8

ADN class 8

Transport labels



14.4. Packing group

1,5,7-Triazabicyclo(4.4.0)dec-5-ene (1,3,4,6,7,8-hexahydro-2H-pyrimido(1,2-a)pyrimidine)

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

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-B
ADR transport category	2
Emergency Action Code	2X
Hazard Identification Number (ADR/RID)	80
Tunnel restriction code	(E)

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

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	Not applicable.

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.

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

1,5,7-Triazabicyclo(4.4.0)dec-5-ene (1,3,4,6,7,8-hexahydro-2H-pyrimido(1,2-a)pyrimidine)

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	Eye Dam. = Serious eye damage Skin Corr. = Skin corrosion
Classification procedures according to SI 2019 No. 720	Eye Dam. 1 - H318: Skin Corr. 1B - H314: : Expert judgement.
Training advice	Only trained personnel should use this material.
Revision date	28/07/2022
Revision	1
SDS number	1246
Hazard statements in full	H314 Causes severe skin burns and eye damage. H318 Causes serious eye damage.

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.