Safety Data Sheet
acc. to OSHA HCS

Date of issue: 06/26/2026 Revision date 06/26/2026

1 Identification

· **Product identifier**

· **Trade name: Mtb ATP Synthase-IN-1**
· **Synonym**
3-(Benzo[d][1,3]dioxol-5-ylamino)-4-((pyridin-2-ylmethyl)amino)cyclobut-3-ene-1,2-dione
C17H13N3O4
· **Other means of identification**

· **Article number:** 46247
· **Application of the substance / the mixture**
This product is for research use - Not for human or veterinary diagnostic or therapeutic use.

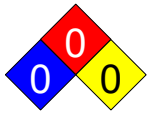
· **Details of the supplier of the safety data sheet**
· **Manufacturer/Supplier:**
Cayman Chemical Co.
1180 E. Ellsworth Rd.
Ann Arbor, MI 48108
USA

· **Information department:** Product safety department
· **Emergency telephone number:**
During normal opening times: +1 (734) 971-3335
US/CANADA: 800-424-9300
Outside US/CANADA: 703-741-5970

2 Hazard(s) identification

· **Classification of the substance or mixture**
The substance is not classified, according to the Globally Harmonized System (GHS).

· **Label elements**
· **GHS label elements** None
· **Hazard pictograms** None
· **Signal word** None
· **Hazard statements** None
· **Information pertaining to particular dangers for man and environment:**
· **Classification system:**
· **NFPA ratings (scale 0 - 4)**



Health = 0
Fire = 0
Reactivity = 0

· **HMIS-ratings (scale 0 - 4)**



Health = 0
Fire = 0
Reactivity = 0

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· **Other hazards**
· **Results of PBT and vPvB assessment**
· **PBT:** Not applicable
· **vPvB:** Not applicable
· **Classification according to (d)(1)(ii) of § 1910.1200**
The SDS issuer does not object to the classifications provided by importers or manufacturers of precursor products.
· **Hazards not otherwise classified**
There are no adverse physical or health effects known that are not covered by the hazard classes of the Hazard Communications Standard.

3 Composition/information on ingredients

· **Chemical characterization: Substances**
· **CAS No. Description**
Mtb ATP Synthase-IN-1

4 First-aid measures

· **Description of first aid measures**
· **General information:** No special measures required.
· **After inhalation:** Supply fresh air; consult doctor in case of complaints.
· **After skin contact:** Generally the product does not irritate the skin.
· **After eye contact:** Rinse opened eye for several minutes under running water.
· **After swallowing:** If symptoms persist consult doctor.
· **Most important symptoms and effects, both acute and delayed**
No further relevant information available.
· **Indication of any immediate medical attention and special treatment needed**
No further relevant information available.

5 Fire-fighting measures

· **Extinguishing media**
· **Suitable extinguishing agents:**
Use fire fighting measures that suit the environment.
A solid water stream may be inefficient.
· **Special hazards arising from the substance or mixture** No further relevant information available.
· **Advice for firefighters**
· **Protective equipment:** No special measures required.

6 Accidental release measures

· **Personal precautions, protective equipment and emergency procedures** Not required
· **Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
· **Methods and material for containment and cleaning up:** Pick up mechanically.
· **Protective Action Criteria for Chemicals**
· **PAC-1:** Substance is not listed.
· **PAC-2:** Substance is not listed.
· **PAC-3:** Substance is not listed.

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· **Reference to other sections**
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

7 Handling and storage

· **Precautions for safe handling** No special measures required.
· **Information about protection against explosions and fires:** No special measures required.

· **Conditions for safe storage, including any incompatibilities**
· **Storage:** Store in accordance with information listed on the product insert.
· **Requirements to be met by storerooms and receptacles:** No special requirements.
· **Information about storage in one common storage facility:** Not required
· **Further information about storage conditions:** None.
· **Specific end use(s)** No further relevant information available.

8 Exposure controls/personal protection

· **Control parameters**
· **Components with limit values that require monitoring at the workplace:** Not required.
· **Additional information:** The lists that were valid during the creation were used as basis.

· **Exposure controls**
· **Appropriate engineering controls** No further data; see section 7.
· **Personal protective equipment:**
· **General protective and hygienic measures:**
The usual precautionary measures for handling chemicals should be followed.
· **Breathing equipment:** Not required
· **Protection of hands:**
The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.
Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.
Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation
· **Material of gloves**
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.
· **Penetration time of glove material**
The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.
· **Eye protection:** Not required

9 Physical and chemical properties

· **Information on basic physical and chemical properties**
· **General Information**

· **Physical state**	Solid
· **Color:**	Not determined
· **Odor:**	Characteristic
· **Structural Formula**	C17H13N3O4

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· **Molecular Weight**	323.3 g/mol
· **Storage Buffer**	
· **Odor threshold:**	Not determined
· **Formulation**	
· **Melting point/Melting range:**	Undetermined
· **Boiling point/Boiling range:**	Undetermined
· **Flammability:**	Product is not flammable.
· **Explosion limits:**	
· **Lower:**	Not determined
· **Upper:**	Not determined
· **Flash point:**	Not applicable
· **Decomposition temperature:**	Not determined
· **pH-value:**	Not applicable
· **Viscosity:**	
· **Kinematic:**	Not applicable
· **SOLUBILITY**	
· **Dynamic:**	Not applicable
· **Solubility in / Miscibility with**	
· **Water:**	Not determined
· **Partition coefficient (n-octanol/water):**	Not determined
· **Vapor pressure:**	Not applicable
· **Vapor pressure:**	
· **Density:**	Not determined
· **Relative density**	Not determined
· **Vapor density**	Not applicable
· **Particle characteristics**	Not determined

· **Other information**	
· **Appearance:**	
· **Form:**	Solid
· **Important information on protection of health and environment, and on safety.**	
· **Ignition temperature:**	Not determined
· **Danger of explosion:**	Product does not present an explosion hazard.
· **Change in condition**	
· **Evaporation rate**	Not applicable.

10 Stability and reactivity

· **Reactivity** No further relevant information available.
· **Chemical stability**
· **Thermal decomposition / conditions to be avoided:**
No decomposition if used according to specifications.
· **Possibility of hazardous reactions** No dangerous reactions known.
· **Conditions to avoid** No further relevant information available.
· **Incompatible materials:** No further relevant information available.
· **Hazardous decomposition products:** No dangerous decomposition products known.

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11 Toxicological information

· **Information on toxicological effects**
· **Acute toxicity:**
· **Primary irritant effect:**
· **on the skin:** No irritant effect.
· **on the eye:** No irritating effect.
· **Sensitization:** No sensitizing effects known.
· **Additional toxicological information:**
When used and handled according to specifications, the product does not have any harmful effects according to our experience and the information provided to us.
The substance is not subject to classification.
· **Interactive effects** No interactive effects between components are known.

· **Carcinogenic categories**
· **IARC (International Agency for Research on Cancer)** Substance is not listed.
· **NTP (National Toxicology Program)** Substance is not listed.
· **OSHA-Ca (Occupational Safety & Health Administration)** Substance is not listed.
· **Alternative sources for toxicological information**
No non-standard sources for toxicological information where used.

12 Ecological information

· **Toxicity**
· **Aquatic toxicity:** No further relevant information available.
· **Persistence and degradability** No further relevant information available.
· **Bioaccumulative potential** No further relevant information available.
· **Mobility in soil** No further relevant information available.
· **Results of PBT and vPvB assessment**
· **PBT:** Not applicable
· **vPvB:** Not applicable
· **Other adverse effects**
· **Additional ecological information:**
· **General notes:**
Water hazard class 1 (Self-assessment): slightly hazardous for water
Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

13 Disposal considerations

· **Waste treatment methods**
· **Recommendation:** Smaller quantities can be disposed of with household waste.

· **Uncleaned packagings:**
· **Recommendation:** Disposal must be made according to official regulations.

14 Transport information

· **UN-Number**
· **DOT, IMDG, IATA** not regulated

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· **UN proper shipping name** · **DOT, IMDG, IATA**	not regulated
· **Transport hazard class(es)** · **DOT, ADN, IMDG, IATA** · **Class**	not regulated
· **Packing group** · **DOT, IMDG, IATA**	not regulated
· **Environmental hazards:**	Not applicable
· **Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code**	Not applicable
· **Special precautions for user**	Not applicable
· **UN "Model Regulation":**	not regulated

15 Regulatory information

· **Safety, health and environmental regulations/legislation specific for the substance or mixture**
· **Sara**
· **Section 355 (extremely hazardous substances):** Substance is not listed.
· **Section 313 (Specific toxic chemical listings):** Substance is not listed.
· **TSCA (Toxic Substances Control Act):** Substance is not listed.
· **Hazardous Air Pollutants** Substance is not listed.
· **Chemicals known to cause cancer:** Substance is not listed.
· **Chemicals known to cause reproductive toxicity for females:** Substance is not listed.
· **Chemicals known to cause reproductive toxicity for males:** Substance is not listed.
· **Chemicals known to cause developmental toxicity:** Substance is not listed.

· **Carcinogenic categories**
· **EPA (Environmental Protection Agency)** Substance is not listed.
· **TLV (Threshold Limit Value)** Substance is not listed.
· **NIOSH-Ca (National Institute for Occupational Safety and Health)** Substance is not listed.
· **Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

16 Other information

· **Department issuing SDS:** Environment protection department.
· **Contact:** -
· **Date of preparation** 06/26/2026
· **Abbreviations and acronyms:**
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
CAS: Chemical Abstracts Service (division of the American Chemical Society)
NFPA: National Fire Protection Association (USA)
HMIS: Hazardous Materials Identification System (USA)
PBT: Persistent, Bioaccumulative and Toxic
vPvB: very Persistent and very Bioaccumulative
NIOSH: National Institute for Occupational Safety
OSHA: Occupational Safety & Health
TLV: Threshold Limit Value
PEL: Permissible Exposure Limit
REL: Recommended Exposure Limit