



SAFETY DATA SHEET

DRAFT FOR TECHNICAL AND REGULATORY REVIEW

Product name	2-(4-Isothiocyanatobenzyl)-1,4,7-triazacyclononane-1,4,7-triacetic acid
Product code	Pending verification by Comora before issue. Catalog record: KML-000238
CAS number	147597-66-8
SDS version	0.1 - Unapproved draft
Issue date	2026-10-02 - draft preparation only
Supersedes	Initial draft; no approved version

Supplier-source draft. Sections 4-14 use the US source SDS; section 2 also shows the EU classification where available. Product equivalence and EU/US requirements must be verified before issue.

SECTION 1 IDENTIFICATION

1.1 Product identifier	2-(4-Isothiocyanatobenzyl)-1,4,7-triazacyclononane-1,4,7-triacetic acid
Other means of identification	CAS: 147597-66-8; Formula: C ₂₀ H ₂₆ N ₄ O ₆ S; Molecular weight: 450.51 g/mol. Source SDS name: 2,2',2''-(2-(4-Isothiocyanatobenzyl)-1,4,7-triazonane-1,4,7-triyl)triacetic acid. Chemical form and stereochemistry require product confirmation.
1.2 Recommended use	Intended Comora uses: pending verification. Source use: The end use(s) have not been fully determined. The substance is supplied for Research and Development purposes by professionals only.
Restrictions on use	Restrictions on use: pending product-specific verification. Not an authorization for medical or consumer use.
1.3 Supplier	Tianjin Comora Technology Co., Ltd.
Address	Pending verification by Comora before issue.
Telephone	+86 15908635794 (business contact; not a verified emergency line)
WhatsApp	+86 15908635794
Email	tao@comoratj.com
Website	www.comoratj.com
1.4 Emergency telephone	Pending verification by Comora before issue. Business contacts above must not be treated as a 24-hour emergency service.

SECTION 2 HAZARDS IDENTIFICATION

2.1 GHS classification	US supplier SDS: Acute toxicity, oral (Category 3) H301 Skin corrosion/irritation (Category 2) H315 Serious eye damage/eye irritation(Category 2A) H319 Sensitisation, respiratory(Category 1, 1A, 1B) H334 Specific target organ toxicity, single exposure;Respiratory system(Category 3) H335 EU supplier SDS: Physical hazards Based on available data, the classification criteria are not met Health hazards Acute toxicity, oral Category 3 (H301) Skin corrosion/irritation Category 2 (H315) Serious eye damage/eye irritation Category 2A (H319) Sensitisation, respiratory Category 1, 1A, 1B (H334) Specific target organ toxicity, single exposure;Respiratory system Category 3 (H335) Environmental hazards Based on available data, the classification criteria are not met Final Comora classification: pending review.
2.2 Signal word	Danger



GHS pictograms	GHS06 - Skull and crossbones; GHS08 - Health hazard 
Hazard statements	H301 Toxic if swallowed H315 Causes skin irritation H319 Causes serious eye irritation H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled H335 May cause respiratory irritation
Precautionary statements	P261 Avoid breathing dust/fume/gas/mist/vapours/spray. P264 Wash hands thoroughly after handling. P270 Do not eat, drink or smoke when using this product. P271 Use only outdoors or in a well-ventilated area. P280 Wear protective gloves/protective clothing/eye protection/face protection. P284 Wear respiratory protection. P301+P310+P330 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. Rinse mouth. P302+P352 IF ON SKIN: Wash with plenty of soap and water. P304+P340+P312 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/physician if you feel unwell. P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P332+P313 If skin irritation occurs: Get medical advice/attention. P337+P313 If eye irritation persists: Get medical advice/attention. Component Concentration 2,2',2''-(2-(4-Isothiocyanatobenzyl)-1,4,7-triazonane-1,4,7-triyl)triacetic acid CAS Number 147597-66-8 - P342+P311 If experiencing respiratory symptoms: Call a POISON CENTER or doctor/physician. P362+P364 Take off contaminated clothing and wash it before reuse. P403+P233 Store in a well-ventilated place. Keep container tightly closed. P405 Store locked up. P501 Dispose of contents/container to in accordance with local regulation
2.3 Other hazards	Additional precautionary phrases are located throughout the safety data sheet.
Unknown acute toxicity	Not determined for the Comora product.

SECTION 3 COMPOSITION INFORMATION ON INGREDIENTS

3.1 Substance or mixture: Substance identity as listed in the catalog; actual supplied composition and chemical form pending verification.

Chemical name	CAS No.	EC No.	Concentration	GHS classification
2-(4-Isothiocyanatobenzyl)-1,4,7-triazacyclononane-1,4,7-triacetic acid	147597-66-8	Not verified	Not verified; catalog purity is not composition	See section 2; supplier-source classification only

Impurities and stabilizing additives: Not reported for the Comora product; review required.

Trade secret statement: No trade-secret claim assessed.

SECTION 4 FIRST AID MEASURES

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

Skin contact: Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

Eye contact: Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

Ingestion: Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects: The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Immediate medical attention and special treatment: No data available General advice: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.



SECTION 5 FIREFIGHTING MEASURES

5.1 Suitable extinguishing media	alcohol-resistant foam, dry chemical or carbon dioxide
Unsuitable extinguishing media	no data
5.2 Specific hazards	In combustion toxic fumes may form.
Hazardous combustion products	Carbon monoxide , carbon dioxide , nitrogen oxides , oxides of sulfur
5.3 Firefighter protection	Wear self-contained breathing apparatus. Wear protective clothing to prevent contact with skin and eyes.

SECTION 6 ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions	Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. Do not attempt to take action without suitable protective clothing. For personal protection see section 8.
Protective equipment	See section 8.
Emergency procedures	See personal precautions above.
6.2 Environmental precautions	Prevent further leakage or spillage if safe to do so. Do not let product enter drains or river. Alert the neighbourhood to the presence of fumes or gas.
6.3 Containment and cleanup	Mix with sand or vermiculite. Sweep up and shovel. Transfer to a closable, labelled salvage container for disposal by an appropriate method.
6.4 Reference to other sections	For disposal see section 13.

SECTION 7 HANDLING AND STORAGE

7.1 Safe handling	Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Wash hands thoroughly after handling. Ensure there is sufficient ventilation of the area. Normal measures for preventive fire protection. For precautions see section 2.2.
7.2 Safe storage	Keep container tightly closed in a dry and well-ventilated area. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Inert atmosphere, 2-8°C
Incompatible materials	No data available
7.3 Specific end use	The end use(s) have not been fully determined. The substance is supplied for Research and Development purposes by professionals only.

SECTION 8 EXPOSURE CONTROLS PERSONAL PROTECTION

8.1 Control parameters

Component	CAS No.	Limit type	Value	Basis / jurisdiction
2-(4-Isothiocyanatobenzyl)-1,4,7-triazacyclononane-1,4,7-triacetic acid	147597-66-8	Not established	Not established	Supplier statement: Contains no substances with occupational exposure limit values. Current EU/US limits require review.



8.2 Exposure controls

Engineering controls	Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
Eye and 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 and hand 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. 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	Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full- face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).
Environmental controls	Do not let product enter drains.

SECTION 9 PHYSICAL AND CHEMICAL PROPERTIES

Property	Value	Property	Value
Physical state	No data available.	Color	No data available.
Appearance	Solid	Odor	No data available
Odor threshold	No data available	pH	No data available
Melting/freezing point	No data available	Boiling point/range	No data available
Flash point	No data available	Evaporation rate	No data available
Flammability	No data available.	Explosive limits	No data available.
Vapor pressure	No data available	Vapor density	No data available
Relative density	No data available	Bulk density	No data available.
Solubility	No data available	Partition coefficient	No data available.
Auto-ignition temperature	No data available	Decomposition temperature	No data available
Kinematic viscosity	No data available.	Dynamic viscosity	No data available.
Particle characteristics	No data available.	Other information	Explosive properties: No data available Oxidizing properties: No data available

SECTION 10 STABILITY AND REACTIVITY

10.1 Reactivity	No data available
10.2 Chemical stability	Stable under recommended storage conditions.



10.3 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	Carbon monoxide , carbon dioxide , nitrogen oxides , oxides of sulfur

SECTION 11 TOXICOLOGICAL INFORMATION

11.1 Likely routes of exposure	No data available.
Symptoms	The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11
Immediate and delayed effects	No data available.

Endpoint	Result	Species	Method / source
Acute oral toxicity	Not reported	Not reported	Not reported
Acute dermal toxicity	Not reported	Not reported	Not reported
Acute inhalation toxicity	Not reported	Not reported	Not reported
Other endpoint	No data available	Not reported	Supplier SDS section 11

Skin corrosion or irritation: No data available

Serious eye damage or irritation: No data available

Respiratory or skin sensitization: No data available

Germ cell mutagenicity: No data available

Carcinogenicity: No data available

Reproductive toxicity: No data available

STOT single exposure: No data available

STOT repeated exposure: No data available

Aspiration hazard: No data available

NTP, IARC, or OSHA carcinogen listing: Not independently verified for current US listings. Additional supplier information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known. No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH

SECTION 12 ECOLOGICAL INFORMATION

Endpoint	Result	Organism	Duration / method
Aquatic toxicity	No data available	Not reported	Not reported
Other ecotoxicity	Not reported	Not reported	Not reported

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 Other adverse effects	No data available PBT/vPvB: No data available Endocrine-disrupting properties: not established.



SECTION 13 DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods	Consult state, local or national regulations for proper disposal. Hand over to authorised disposal company as hazardous waste.
Contaminated packaging	Disposal must be made according to official regulations.
Disposal precautions	Product-specific waste classification and applicable jurisdiction requirements must be verified.

SECTION 14 TRANSPORT INFORMATION

Information	ADR/RID	IMDG	IATA/ICAO	Other
UN number	2811	2811	2811	US DOT: not verified
Proper shipping name	Toxic solid, organic, n.o.s.	Toxic solid, organic, n.o.s.	Toxic solid, organic, n.o.s.	US DOT: not verified
Hazard class	6.1	6.1	6.1	US DOT: not verified
Packing group	III	III	III	US DOT: not verified
Environmental hazards	Not specified in source	Not specified in source	Not specified in source	US DOT: not verified
Special precautions	No special precautions required	No special precautions required	No special precautions required	US DOT: not verified

14.7 Maritime transport in bulk: Not determined. Source transport information must be reviewed for the actual shipment and current mode-specific rules.

SECTION 15 REGULATORY INFORMATION

15.1 Product-specific regulations	United States: OSHA HCS review pending. European Union: CLP and REACH Annex II review pending. This draft is not a declaration of compliance.
Chemical inventories	TSCA, REACH registration and destination-market inventories: not verified.
Restricted substance status	SVHC, restrictions and authorization status: not verified.
15.2 Chemical safety assessment	Not performed or not supplied by Comora.

SECTION 16 OTHER INFORMATION

Preparation / revision date	2026-10-02 (draft preparation; not an effective issue date)
Version / prepared by	0.1 - preparer to be designated by Comora
Approved by	Pending verification by Comora before issue.
Revision summary	Initial source-based review draft. Molecular formula differs between the supplied/BLD record and PubChem. Verify chemical form and stoichiometry before issue. Catalog and source product names use different wording. Confirm synonym equivalence, stereochemistry and salt/solvate state before applying source safety data.



References / abbreviations

BLD Pharmatech: Safety Data Sheet BD01432349 (US); revision 08/16/2025; accessed 2026-10-02. <https://file.bldpharm.com/static/upload/prosds/bldsds-us/1433/SDS-BD01432349.pdf>
BLD Pharmatech: Safety Data Sheet BD01432349 (EU); revision 08/16/2025; accessed 2026-10-02. <https://file.bldpharm.com/static/upload/prosds/bldsds-ger/1433/SDS-BD01432349.pdf>
Identity cross-check only: <https://pubchem.ncbi.nlm.nih.gov/compound/3036142>; accessed 2026-10-02.

Disclaimer

Unapproved technical draft. Supplier information relates to the referenced supplier product and is not proof of equivalence to the material supplied by Tianjin Comora. A qualified person must verify identity, composition, classification, handling measures, transport, company contacts and destination-market requirements before issue. Missing information does not mean absence of hazard. Do not use this draft as a release document.

Template reference

Sixteen-section format retained. OSHA HCS, EU CLP and REACH review is required before issue. Abbreviations: GHS, Globally Harmonized System; ADR/RID, European road/rail transport; IMDG, maritime transport; IATA, air transport; PBT/vPvB, persistence and bioaccumulation criteria.