

Chemical Safety Data Sheet MSDS / SDS

3-CARBOXYPHENYL ISOTHIOCYANATERevision Date:2026-05-31 Revision Number:1

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

Product name : 3-CARBOXYPHENYL ISOTHIOCYANATE
CBnumber : CB5449192
CAS : 2131-63-7
Synonyms : 3-Carboxyphenyl isothiocyanate,3-isothiocyanatobenzoic acid

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

Precautionary statements

P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P405 Store locked up.

Hazard statements

H302 Harmful if swallowed

H312 Harmful in contact with skin

H331 Toxic if inhaled

H318 Causes serious eye damage

H314 Causes severe skin burns and eye damage

SECTION 3: Composition/information on ingredients

Substance

Product name	: 3-CARBOXYPHENYL ISOTHIOCYANATE
Synonyms	: 3-Carboxyphenyl isothiocyanate,3-isothiocyanatobenzoic acid
CAS	: 2131-63-7
MF	: C8H5NO2S
MW	: 179.2

SECTION 4: First aid measures

General Advice

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.

Keep eye wide open while rinsing.

Skin Contact

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Call a physician immediately.

Inhalation

Remove to fresh air. If not breathing, give artificial respiration. Call a physician or poison control center immediately. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device.

Ingestion

Immediate medical attention is required. Do NOT induce vomiting. Drink plenty of water. Never give anything by mouth to an unconscious person.

Most important symptoms and effects

Causes burns by all exposure routes. Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

Notes to Physician

Treat symptomatically.

SECTION 5: Firefighting measures

Suitable Extinguishing Media

CO₂, dry chemical, dry sand, alcohol-resistant foam.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

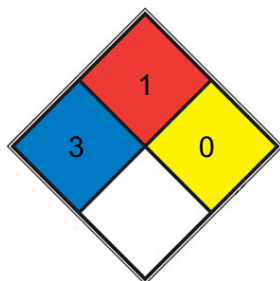
The product causes burns of eyes, skin and mucous membranes.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

Thermal decomposition can lead to release of irritating gases and vapors.

NFPA 704



■ HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

■ FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N₂](#))

□ SPEC.
HAZ.

SECTION 6: Accidental release measures

Personal Precautions

Use personal protective equipment as required. Evacuate personnel to safe areas. Avoid contact with skin, eyes or clothing.

Environmental Precautions

Should not be released into the environment. Do not allow material to contaminate ground water system. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

Sweep up and shovel into suitable containers for disposal. Avoid dust formation.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: Handling and storage

Handling

Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe dust. Do not ingest. If swallowed then seek immediate medical assistance.

Storage

Air sensitive. Corrosives area. Keep containers tightly closed in a dry, cool and well-ventilated place.

Specific Use(s)

Use in laboratories

SECTION 8: Exposure controls/personal protection

Control Parameters

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

Exposure Controls

Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

Personal protective equipment

Eye Protection

Goggles (European standard - EN 166)

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.

(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection

Long sleeved clothing

Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Recommended Filter type: Particulates filter conforming to EN 143

Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Particle filtering: EN149:2001

When RPE is used a face piece Fit Test should be conducted

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls

No information available.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Light brown

Physical State

Solid

Odor

Irritating

Odor Threshold

No data available

pH

No information available

Melting Point/Range

~ 165 °C / 329 °F

Softening Point

No data available

Boiling Point/Range

381.2±25.0 °C(Predicted)

Flash Point

No information available

Method - No information available

Evaporation Rate

Not applicable Solid

Flammability (solid,gas)

No information available

Explosion Limits

No data available

Vapor Pressure

No data available

Vapor Density

Not applicable Solid

Specific Gravity / Density

1.3522 (rough estimate)

Bulk Density

1.3522 (rough estimate)

Water Solubility

100.4mg/L(25 °C)

Solubility in other solvents

No information available

Partition Coefficient (n-octanol/water)

No data available

Autoignition Temperature

No data available

Decomposition Temperature

No data available

Viscosity

Not applicable Solid

Explosive Properties

No information available

Oxidizing Properties

No information available

Molecular Formula

C8 H5 N O2 S

Molecular Weight

179.20

SECTION 10: Stability and reactivity

Stability

Moisture sensitive.

Hazardous Reactions

None under normal processing.

Hazardous Polymerization

No information available.

Conditions to Avoid

Exposure to light.

Materials to avoid

No information available.

Hazardous Decomposition Products

None under normal use conditions.

SECTION 11: Toxicological information

Product Information

(a) acute toxicity;

(b) skin corrosion/irritation;

Category 1 B

(c) serious eye damage/irritation;

Category 1

(d) respiratory or skin sensitization;

Respiratory

No data available

Skin

No data available

(e) germ cell mutagenicity;

No data available

(f) carcinogenicity;

No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity;

No data available

(h) STOT-single exposure;

No data available

(i) STOT-repeated exposure;

No data available

Target Organs

No information available.

(j) aspiration hazard;

Not applicable

Solid

Symptoms / effects,both acute and delayed

Product is a corrosive material. Use of gastric lavage or emesis is contraindicated.

Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

SECTION 12: Ecological information

Ecotoxicity effects

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

Persistence and Degradability

No information available

Bioaccumulative Potential

No information available

Mobility in soil

No information available

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

Persistent Organic Pollutant

This product does not contain any known or suspected substance

Ozone Depletion Potential

This product does not contain any known or suspected substance

SECTION 13: Disposal considerations

Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains. Do not flush to sewer. Large amounts will affect pH and harm aquatic organisms.

SECTION 14: Transport information

Road and Rail Transport

UN-No

UN2923

Proper Shipping Name

Corrosive solid, toxic, n.o.s.

Technical Shipping Name

(3-Carboxyphenyl isothiocyanate)

Hazard Class

8

Subsidiary Hazard Class

6.1

Packing Group

III

IMDG/IMO

UN-No

UN2923

Proper Shipping Name

Corrosive solid, toxic, n.o.s.

Technical Shipping Name

(3-Carboxyphenyl isothiocyanate)

Hazard Class

8

Subsidiary Hazard Class

6.1

Packing Group

III

IATA

UN-No

UN2923

Proper Shipping Name

CORROSIVE SOLID, TOXIC, N.O.S.*

Technical Shipping Name

(3-Carboxyphenyl isothiocyanate)

Hazard Class

8

Subsidiary Hazard Class

6.1

Packing Group

III

Special Precautions for User

No special precautions required

SECTION 15: Regulatory information

International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

National Regulations

SECTION 16: Other information

Prepared By

Revision Date

24-Oct-2025

Revision Summary

Not applicable.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene. Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Legend

CAS

Chemical Abstracts Service

TSCA

United States Toxic Substances Control Act Section 8(b)

Inventory

EINECS/ELINCS

European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

DSL/NDSL

Canadian Domestic Substances List/Non-Domestic Substances List

PICCS

Philippines Inventory of Chemicals and Chemical Substances

ENCS

Japanese Existing and New Chemical Substances

IECSC

Chinese Inventory of Existing Chemical Substances

AICS

Australian Inventory of Chemical Substances

KECL

Korean Existing and Evaluated Chemical Substances

NZIoC

New Zealand Inventory of Chemicals

WEL

Workplace Exposure Limit

TWA

Time Weighted Average

ACGIH

American Conference of Governmental Industrial Hygienists

IARC

International Agency for Research on Cancer

DNEL

Derived No Effect Level

PNEC

Predicted No Effect Concentration

RPE

Respiratory Protective Equipment

LD50

Lethal Dose 50%

LC50

Lethal Concentration 50%

EC50

Effective Concentration 50%

NOEC

No Observed Effect Concentration

POW

Partition coefficient Octanol:Water

PBT

Persistent, Bioaccumulative, Toxic

vPvB

very Persistent, very Bioaccumulative

ICAO/IATA

International Civil Aviation Organization/International Air
Transport Association

IMO/IMDG

International Maritime Organization/International Maritime
Dangerous Goods Code

ADR

European Agreement Concerning the International Carriage of
Dangerous Goods by Road

MARPOL

International Convention for the Prevention of Pollution from
Ships

OECD

Organisation for Economic Co-operation and Development

ATE

Acute Toxicity Estimate

BCF

Bioconcentration factor

VOC

(Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The 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, unless specified in the text

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.