

Chemical Safety Data Sheet MSDS / SDS

1-(2-Chlorophenyl)-2-thiourea

Revision Date:2024-12-21 Revision Number:1

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

Product name : 1-(2-Chlorophenyl)-2-thiourea
CBnumber : CB4106438
CAS : 5344-82-1
EINECS Number : 226-291-6
Synonyms : 1-(2-CHLOROPHENYL)THIOUREA, 1-(2-Chlorophenyl)-2-thiourea

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 : 400-158-6606

SECTION 2: Hazards identification**Classification of the substance or mixture**

Acute toxicity - Category 2, Oral

Skin irritation, Category 2

Skin sensitization, Category 1

Label elements**Pictogram(s)**

□

Signal word Danger

Hazard statement(s)

H300 Fatal if swallowed

Precautionary statement(s)

P330 Rinse mouth.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

P302+P350 IF ON SKIN: Gently wash with plenty of soap and water.

Prevention

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P272 Contaminated work clothing should not be allowed out of the workplace.

Response

P301+P316 IF SWALLOWED: Get emergency medical help immediately.

P321 Specific treatment (see ... on this label).

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P332+P317 If skin irritation occurs: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

P333+P317 If skin irritation or rash occurs: Get medical help.

Storage

P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: 1-(2-Chlorophenyl)-2-thiourea
Synonyms	: 1-(2-CHLOROPHENYL)THIOUREA, 1-(2-Chlorophenyl)-2-thiourea
CAS	: 5344-82-1
EC number	: 226-291-6
MF	: C7H7ClN2S
MW	: 186.66

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately.

Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms and effects, both acute and delayed

High oral toxicity. (EPA, 1998)

Indication of any immediate medical attention and special treatment needed

no data available

SECTION 5: Firefighting measures

Extinguishing media

Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]: SMALL FIRE: Dry chemical, CO₂ or water spray. LARGE FIRE: Dry chemical, CO₂, alcohol-resistant foam or water spray. Move containers from fire area if you can do it without risk. Dike fire-control water for later disposal; do not scatter the material. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Do not get water inside containers. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. (ERG, 2016)

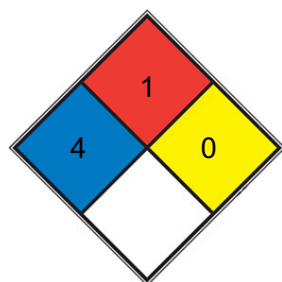
Specific Hazards Arising from the Chemical

When heated to decomposition it emits very toxic fumes of chlorides, nitrogen oxides, and sulfur oxides. (EPA, 1998)

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

NFPA 704



■ HEALTH	4	Very short exposure could cause death or major residual injury (e.g. hydrogen cyanide, phosgene, methyl isocyanate, hydrofluoric 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, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The

selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	Thiourea, (2-chlorophenyl)- is a needles or plates. Used as an herbicide. Not registered as a pesticide in the U.S. (EPA, 1998)
Colour	NEEDLES OR PLATES
Odour	no data available
Melting point/freezing point	144-149°C
Boiling point or initial boiling point and boiling range	293.1°C at 760mmHg
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	131.1°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	VERY SOL IN WATER; SLIGHTLY SOL IN AMMONIA
Partition coefficient n-octanol/water	Estimated log Kow of 1.20.
Vapour pressure	no data available
Density and/or relative density	1.441g/cm3
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

No rapid reaction with air. No rapid reaction with water.

Chemical stability

no data available

Possibility of hazardous reactions

When heated to decomposition it emits very toxic fumes of chlorides, nitrogen oxides, and sulfur oxides. [EPA, 1998]. Organosulfides are

incompatible with acids, diazo and azo compounds, halocarbons, isocyanates, aldehydes, alkali metals, nitrides, hydrides, and other strong reducing agents. Reactions with these materials generate heat and in many cases hydrogen gas. Many of these compounds may liberate hydrogen sulfide upon decomposition or reaction with an acid.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/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

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

no data available

Bioaccumulative potential

Based on an estimated log Kow of 1.20(1), the BCF for 2-chlorophenylthiourea can be estimated to be 4.8 from a recommended regression-derived equation(2, SRC). This indicates that environmental bioconcentration is not significant(SRC).

Mobility in soil

Based on an estimated log Kow of 1.20(1), the Koc for 2-chlorophenylthiourea can be estimated to range from 11-107 using various regression-derived equations(2, SRC); these Koc estimations indicate high to very high soil mobility(3). Although high soil mobility can be predicted from the log Kow value, 2-chlorophenylthiourea may undergo significant adsorption in soil due to a covalent bonding with humic materials(SRC). Secondary amines (such as N-methylaniline) have been observed to undergo covalent bonding with humates(4) an initial rapid (and reversible) bonding phase is followed by a slow reaction (that is not readily reversible) in which the amine compound is chemically altered to yield an amino-substituted quinone(4). This covalent bonding process represents a mechanism in which aromatic amines may be converted to latent form in the biosphere(4).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN2811 (For reference only, please check.)

IMDG: UN2811 (For reference only, please check.)

IATA: UN2811 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (For reference only, please check.)

IMDG: TOXIC SOLID, ORGANIC, N.O.S. (For reference only, please check.)

IATA: TOXIC SOLID, ORGANIC, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

PICCS

Not Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Not Listed.

Korea Existing Chemicals List (KECL)

Not Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pagelD=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Disclaimer:

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