SAFETY DATA SHEET

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

1.1 Product identifiers

Product name: \( N,N' \)-Diphenylthiourea

Product Number: T28355
Brand: Aldrich
CAS-No.: 102-08-9

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

Identified uses: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone: +1 314 771-5765
Fax: +1 800 325-5052

1.4 Emergency telephone

Emergency Phone #: 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Skin sensitization (Category 1), H317
Reproductive toxicity (Category 2), H361
Specific target organ toxicity - repeated exposure (Category 2), H373
Short-term (acute) aquatic hazard (Category 2), H401
Long-term (chronic) aquatic hazard (Category 2), H411

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Warning
Hazard statement(s)

H317  May cause an allergic skin reaction.
H361  Suspected of damaging fertility or the unborn child.
H373  May cause damage to organs through prolonged or repeated exposure.
H411  Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P201  Obtain special instructions before use.
P202  Do not handle until all safety precautions have been read and understood.
P260  Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
P272  Contaminated work clothing must not be allowed out of the workplace.
P273  Avoid release to the environment.
P280  Wear protective gloves/ protective clothing/ eye protection/ face protection.
P302 + P352  IF ON SKIN: Wash with plenty of soap and water.
P308 + P313  IF exposed or concerned: Get medical advice/ attention.
P333 + P313  If skin irritation or rash occurs: Get medical advice/ attention.
P363  Wash contaminated clothing before reuse.
P391  Collect spillage.
P405  Store locked up.
P501  Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms: 1,3-Diphenyl-2-thiourea
           Diphenylsulfourea
           Thiocarbonilide

Formula: C13H12N2S
Molecular weight: 228.31 g/mol
CAS-No.: 102-08-9
EC-No.: 203-004-2

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>N,N’-diphenylthiourea</td>
<td>Skin Sens. 1; Repr. 2; STOT RE 2; Aquatic Acute 2; Aquatic Chronic 2; H317, H361, H373, H401, H411</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

For the full text of the H-Statements mentioned in this Section, see Section 16.
SECTION 4: First aid measures

4.1 Description of first-aid measures

**General advice**
Show this material safety data sheet to the doctor in attendance.

**If inhaled**
After inhalation: fresh air. Call in physician.

**In case of skin contact**
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Consult a physician.

**In case of eye contact**
After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

**If swallowed**
After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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

4.3 Indication of any immediate medical attention and special treatment needed
No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

**Suitable extinguishing media**
Water Foam Carbon dioxide (CO2) Dry powder

**Unsuitable extinguishing media**
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Nitrogen oxides (NOx)
Sulfur oxides
Combustible.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information
Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.
For personal protection see section 8.

6.2 Environmental precautions
Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling
Advice on safe handling
Work under hood. Do not inhale substance/mixture.

Hygiene measures
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Storage conditions
Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class
Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters
Ingredients with workplace control parameters
Contains no substances with occupational exposure limit values.

8.2 Exposure controls
Appropriate engineering controls
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
Personal protective equipment

Eye/face protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

Body Protection
protective clothing

Respiratory protection
required when dusts are generated.
Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure
Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
Form: solid

b) Odor
No data available

c) Odor Threshold
No data available

d) pH
No data available

e) Melting point/freezing point
Melting point/range: 152 - 155 °C (306 - 311 °F) - lit.

f) Initial boiling point and boiling range
> 250 °C > 482 °F - OECD Test Guideline 103

By

g) Flash point
() No data available
h) Evaporation rate: No data available
i) Flammability (solid, gas): No data available
j) Upper/lower flammability or explosive limits: No data available
k) Vapor pressure: No data available
l) Vapor density: No data available
m) Density: 1.32 g/cm³ at 20 °C (68 °F)
   Relative density: No data available
n) Water solubility: 0.02352 g/l at 20 °C (68 °F) - OECD Test Guideline 105
o) Partition coefficient: n-octanol/water
   log Pow: 2.01 - Bioaccumulation is not expected., (External MSDS)
p) Autoignition temperature: No data available
q) Decomposition temperature: No data available
r) Viscosity: No data available
s) Explosive properties: No data available
t) Oxidizing properties: none

9.2 Other safety information
No data available

SECTION 10: Stability and reactivity

10.1 Reactivity
The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
No information available

10.5 Incompatible materials
No data available

10.6 Hazardous decomposition products
In the event of fire: see section 5
SECTION 11: Toxicological information

11.1 Information on toxicological effects

**Acute toxicity**
LD₅₀ Oral - Rat - male and female - > 2,000 mg/kg
Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.
Inhalation: No data available
LD Dermal - Rat - male and female - > 2,000 mg/kg (OECD Test Guideline 402)

**Skin corrosion/irritation**
Skin - Rabbit
Result: slight irritation - 4 h (OECD Test Guideline 404)

**Serious eye damage/eye irritation**
Eyes - Rabbit
Result: slight irritation
(OECD Test Guideline 405)
slight irritation

**Respiratory or skin sensitization**
Patch test: - Human
Result: positive

**Germ cell mutagenicity**
Test Type: reverse mutation assay
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative

Test Type: Micronucleus test
Species: Rat
Cell type: Bone marrow
Application Route: Oral
Method: OECD Test Guideline 474
Result: negative

**Carcinogenicity**
IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA’s list of regulated carcinogens.

**Reproductive toxicity**
Suspected of damaging the unborn child.

**Specific target organ toxicity - single exposure**
No data available

**Specific target organ toxicity - repeated exposure**
May cause damage to organs through prolonged or repeated exposure. Aspiration hazard


11.2 Additional Information
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.
Other dangerous properties cannot be excluded.
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity
Toxicity to fish 
static test LC50 - Danio rerio (zebra fish) - > 33 mg/l - 96 h
(OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates 
static test EC50 - Daphnia magna (Water flea) - 10 mg/l - 48 h
(OECD Test Guideline 202)
Toxicity to algae 
static test - Pseudokirchneriella subcapitata (green algae) - 14 mg/l - 72 h
(OECD Test Guideline 201)
Toxicity to bacteria 
microtox test EC50 - Bacteria - 9,800 mg/l - 15 min
Remarks: (External MSDS)

12.2 Persistence and degradability
Biodegradability 
aerobic - Exposure time 28 d
Result: 0 % - Not readily biodegradable.
(OECD Test Guideline 301F)

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods
Product 
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.
SECTION 14: Transport information

**DOT (US)**
Not dangerous goods

**IMDG**
- UN number: 3077
- Class: 9
- Packing group: III
- EMS-No: F-A, S-F
- Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (N,N'-diphenylthiourea)
- Marine pollutant: yes

**IATA**
- UN number: 3077
- Class: 9
- Packing group: III
- Proper shipping name: Environmentally hazardous substance, solid, n.o.s. (N,N'-diphenylthiourea)

**Further information**
EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids. Packages smaller than or equal to 5 kg / L, not dangerous goods of Class 9.

SECTION 15: Regulatory information

**SARA 302 Components**
This material does not contain any components with a section 302 EHS TPQ.

**SARA 313 Components**
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**
Acute Health Hazard

**Massachusetts Right To Know Components**
No components are subject to the Massachusetts Right to Know Act.
SECTION 16: Other information

Further information
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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