

Propylthiouracil SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- * Product Name: Propylthiouracil
- * Catalog Number: S1988
- * CAS Number: 51-52-5
- * IUPAC Name: 2,3-dihydro-6-propyl-2-thioxo-4(1H)-pyrimidinone

Relevant identified uses and uses advised against

- * Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.
- * Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

- * Company: Selleck Chemicals
- * TollFree: +1 877 796-6397
- * Tel: +1 832 582-8158
- * Fax: +1 832 582-8590

Emergency telephone number

- * Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

- Acute toxicity (oral): Category 4. H302
- Carcinogenicity: Category 1. H350
- Carcinogenicity: Category 2. H351
- Reproductive toxicity: Category 2. H361
- Specific target organ toxicity (repeated exposure): Category 1. H372

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)

- H302: Harmful if swallowed
- H350: May cause cancer
- H351: Suspected of causing cancer
- H361: Suspected of damaging fertility or the unborn child
- H372: Causes damage to organs through prolonged or repeated exposure

Precautionary statement(s)

None.

Prevention	P203: Obtain, read and follow all safety instructions before use. P260: Do not breathe dust/fume/gas/mist/vapors/spray. P264: Wash hands 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.
Response	P301+P317: IF SWALLOWED: Get medical help. P318: if exposed or concerned, get medical advice. P319: Get medical help if you feel unwell. P330: Rinse mouth.
Storage	P405: Store locked up.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: Propylthiouracil

CAS Number: 51-52-5

PubChem CID: 657298

Molecular formula: C₇H₁₀N₂OS

Molecular weight: 170.23 g/mol

IUPAC name: 6-propyl-2-sulfanylidene-1H-pyrimidin-4-one

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air.

IMMEDIATELY call a physician and be prepared to transport the victim to a hospital even if no symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater

Skin contact: SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment.

Eye contact: EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician.

IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.

Ingestion: INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO₂), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. (NTP, 1992)

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 Methods and materials for containment and cleaning up

PRECAUTIONS FOR "CARCINOGENS": A high-efficiency particulate arrestor (HEPA) or charcoal filters can be used to minimize amt of carcinogen in exhausted air ventilated safety cabinets, lab hoods, glove boxes or animal rooms ... Filter housing that is designed so that used filters can be transferred into plastic bag without contaminating maintenance staff is avail commercially. Filters should be placed in plastic bags immediately after removal ... The plastic bag should be sealed immediately ... The sealed bag should be labelled properly ... Waste liquids ... should be placed or collected in proper containers for disposal. The lid should be secured & the bottles properly labelled. Once filled, bottles should be placed in plastic bag, so that outer surface ... is not contaminated ... The plastic bag should also be sealed & labelled. ... Broken glassware ... should be decontaminated by solvent extraction, by chemical destruction, or in specially designed incinerators. /Chemical Carcinogens/

SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations. SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.

PRECAUTIONS FOR "CARCINOGENS": There is no universal method of disposal that has been proved satisfactory for all carcinogenic compounds & specific methods of chem destruction ... published have not been tested on all kinds of carcinogen-containing waste. ... summary of avail methods & recommendations ... /given/ must be treated as guide only. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": ... Incineration may be only feasible method for disposal of contaminated laboratory waste from biological expt. However, not all incinerators are suitable for this purpose. The most efficient type ... is probably the gas-fired type, in which a first-stage combustion with a less than stoichiometric air:fuel ratio is followed by a second stage with excess air. Some ... are designed to accept ... aqueous & organic-solvent solutions, otherwise it is necessary ... to absorb soln onto suitable combustible material, such as sawdust. Alternatively, chem destruction may be used, esp when small quantities ... are to be destroyed in laboratory. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": HEPA (high-efficiency particulate arrestor) filters ... can be disposed of by incineration. For spent charcoal filters, the adsorbed material can be stripped off at high temp & carcinogenic wastes generated by this treatment conducted to & burned in an incinerator. ... LIQUID WASTE: ... Disposal should be carried out by incineration at temp that ... ensure complete combustion. SOLID WASTE: Carcasses of lab animals, cage litter & misc solid wastes ... should be disposed of by incineration at temp high enough to ensure destruction of chem carcinogens or their metabolites. /Chemical Carcinogens/

For more Disposal Methods (Complete) data for PROPYL THIOURACIL (6 total), please visit the HSDB record page.

PRECAUTIONS FOR "CARCINOGENS": Smoking, drinking, eating, storage of food or of food & beverage containers or utensils, & the application of cosmetics should be prohibited in any laboratory. All personnel should remove gloves, if worn, after completion of procedures in which carcinogens have been used. They should ... wash ... hands, preferably using dispensers of liq detergent, & rinse ... thoroughly. Consideration should be given to appropriate methods for cleaning the skin, depending on nature of the contaminant. No standard procedure can be recommended, but the use of organic solvents should be avoided. Safety pipettes should be used for all pipetting. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": In animal laboratory, personnel should remove their outdoor clothes & wear protective suits (preferably disposable, one-piece & close-fitting at ankles & wrists), gloves, hair covering & overshoes. ... Clothing should be changed daily but ... discarded immediately if obvious contamination occurs ... /also,/ workers should shower immediately. In chemical laboratory, gloves & gowns should always be worn ... however, gloves should not be assumed to provide full protection. Carefully fitted masks or respirators may be necessary when working with particulates or gases, & disposable plastic aprons might provide addnl protection. If gowns are of distinctive color, this is a reminder that they should not be worn outside of lab. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": ... Operations connected with synth & purification ... should be carried out under well-ventilated hood. Analytical procedures ... should be carried out with care & vapors evolved during ... procedures should be removed. ... Expert advice should be obtained before existing fume cupboards are used ... & when new fume cupboards are installed. It is desirable that there be means for decreasing the rate of air extraction, so that carcinogenic powders can be handled without ... powder being blown around the hood. Glove boxes should be kept under negative air pressure. Air changes should be adequate, so that concn of vapors of volatile carcinogens will not occur. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": Vertical laminar-flow biological safety cabinets may be used for containment of in vitro procedures ... provided that the exhaust air flow is sufficient to provide an inward air flow at the face opening of the cabinet, & contaminated air plenums that are under positive pressure are leak-tight. Horizontal laminar-flow hoods or safety cabinets, where filtered air is blown across the working area towards the operator, should never be used ... Each cabinet or fume cupboard to be used ... should be tested before work is begun (eg, with fume bomb) & label fixed to it, giving date of test & avg air-flow measured. This test should be repeated periodically & after any structural changes. /Chemical Carcinogens/

For more Preventive Measures (Complete) data for PROPYL THIOURACIL (9 total), please visit the HSDB record page.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

SMALL SPILLS AND LEAKAGE: If you spill this chemical, dampen the solid spill material with 5% ammonium hydroxide, then transfer the dampened material to a suitable container. Use absorbent paper dampened with 5% ammonium hydroxide to pick up any remaining material. Your contaminated clothing and the absorbent paper should be sealed in a vapor-tight plastic bag for eventual disposal. Wash all contaminated surfaces with 5% ammonium hydroxide followed by washing with a soap and water solution. Do not reenter the contaminated area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned.

STORAGE PRECAUTIONS: You should protect this chemical from exposure to light. Keep the container tightly closed under an inert atmosphere, and store under refrigerated temperatures. (NTP, 1992)

Commercially available propylthiouracil tablets should be stored in well-closed containers at a temperature less than 40 °C, preferably between 15-30 °C.

PRECAUTIONS FOR "CARCINOGENS": Storage site should be as close as practical to lab in which carcinogens are to be used, so that only small quantities required for ... expt need to be carried. Carcinogens should be kept in only one section of cupboard, an explosion-proof refrigerator or freezer (depending on chemico-physical properties ...) that bears appropriate label. An inventory ... should be kept, showing quantity of carcinogen & date it was acquired ... Facilities for dispensing ... should be contiguous to storage area. /Chemical Carcinogens/

7.2 Conditions for safe storage, including any incompatibilities

Commercially available propylthiouracil tablets should be stored in well-closed containers at a temperature less than 40 °C, preferably between 15-30 °C.

PRECAUTIONS FOR "CARCINOGENS": Storage site should be as close as practical to lab in which carcinogens are to be used, so that only small quantities required for ... expt need to be carried. Carcinogens should be kept in only one section of cupboard, an explosion-proof refrigerator or freezer (depending on chemico-physical properties ...) that bears appropriate label. An inventory ... should be kept, showing quantity of carcinogen & date it was acquired ... Facilities for dispensing ... should be contiguous to storage area. /Chemical Carcinogens/

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

8.1.2 Appropriate engineering controls

Use in a well-ventilated area. Chemical fume hood recommended for powder handling.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear safety glasses with side shields.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Respiratory protection usually not required under normal use with adequate ventilation.

Use N95 respirator for large-scale powder handling.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- a) Appearance: 6-n-propyl-2-thiouracil appears as odorless white crystalline powder of starch-like appearance. Bitter taste. Saturated solution is neutral or slightly acid to litmus. (NTP, 1992)
- b) Odor: No data available
- c) Odor threshold: No data available
- d) pH: Saturated aq soln is neutral or slightly acid to litmus
- e) Melting point/freezing point: 426 to 430 °F (NTP, 1992)
- f) Initial boiling point and boiling range: No data available
- 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) Relative density: No data available
- n) Water solubility: less than 1 mg/mL at 68 °F (NTP, 1992)
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 0.8
- p) Auto-ignition temperature: No data available
- q) Decomposition temperature: No data available
- r) Viscosity: No data available
- s) Explosive properties: No data available
- t) Oxidizing properties: No data available

9.2 Other information

Topological Polar Surface Area (TPSA): 73.2 Å²

Complexity: 222

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

Avoid strong oxidizing agents, strong acids, and strong bases.

10.5 Incompatible materials

Forms complexes with metals and reacts with sulfhydryl-oxidizing agents

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), Sulfur oxides (SO_x).

See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

No acute toxicity data available.

Skin corrosion/irritation:

No data available.

Serious eye damage/eye irritation:

No data available.

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

No data available.

Carcinogenicity:

May cause cancer (H350).

Reproductive toxicity:

Suspected of damaging fertility or the unborn child (H361).

Specific target organ toxicity (single exposure):

H372

Specific target organ toxicity (repeated exposure):

No data available.

Aspiration hazard:

No data available.

11.2 Additional information**Carcinogen classification:**

Propylthiouracil

Group 2B: Possibly carcinogenic to humans

Volume Sup 7: Overall Evaluations of Carcinogenicity: An Updating of IARC Monographs Volumes 1 to 42, 1987; 440 pages; ISBN 92-832-1411-0 (out of print)

Volume 79: (2001) Some Thyrotropic Agents

2001

2000

2B, possibly carcinogenic to humans. (L135)

Exposure routes:

Well absorbed following oral administration.

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

12. ECOLOGICAL INFORMATION**12.1 Toxicity**

Propyl thiouracil's production and use as thyroid inhibitor may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of 6.9×10^{-8} mm Hg at 25 °C indicates propyl thiouracil will exist solely in the particulate phase in the ambient atmosphere. Particulate-phase propyl thiouracil will be removed from the atmosphere by wet and dry deposition. Propyl thiouracil absorbs light >290 nm and may be susceptible to direct photolysis in air. If released to soil, propyl thiouracil is expected to have very high mobility based upon an estimated Koc of 23. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 1.1×10^{-9} atm-cu m/mole. Propyl thiouracil is not expected to volatilize from dry soil surfaces based upon the estimated vapor pressure. Propyl thiouracil was not degraded in a screening study using an activated sludge inoculum over a 28 day incubation period, suggesting biodegradation will be slow in the environment. If released into water, propyl thiouracil is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. BCF values in the range of <2 to <4 measured in fish suggest bioconcentration in aquatic organisms is low. Hydrolysis is not expected to be an important enviro

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 0.8

Low potential for bioaccumulation (Log P < 3).

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available.

12.6 Other adverse effects

No other adverse ecological effects identified.

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods**

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION**14.1 UN number**

Not regulated as dangerous goods (research quantities typically exempt).

14.2 UN proper shipping name

Not subject to transport regulations (small quantities for research use).

14.3 Transport hazard class(es)

Not classified as dangerous goods for transport (research quantities).

14.4 Packing group

Not applicable (not regulated as dangerous goods in typical research quantities).

14.5 Environmental hazards

Marine pollutant: No (not classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable.

15. REGULATORY INFORMATION**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

US EPA / TSCA: Subject to EPA TSCA regulations

EU ECHA / REACH: Not available in public databases.

SARA 302 Components:

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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 (short-term) health hazard

Chronic (long-term) health hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

California Prop. 65 Components:

This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

Other regulatory listings:

- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Carcinogenicity; Developmental Toxicity Authoritative List - IARC Carcinogens - 2B; NTP RoC - reasonable; Prop 65 Report - regardless of intended function of ingredient in the product

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/08

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product.

Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.