Myclobutanil SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Myclobutanil
* Catalog Number: S5704
* CAS Number: 88671-89-0
* IUPAC Name: 1H-1,2,4-Triazole-1-propanenitrile, α-butyl-α-(4-chlorophenyl)-

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
Serious eye irritation: Category 2. H319
Reproductive toxicity: Category 2. H361
Specific target organ toxicity (repeated exposure): Category 2. H373
Chronic aquatic toxicity: Category 2. H411

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)	
Signal Word	Warning
Hazard statement(s)	H302: Harmful if swallowed H319: Causes serious eye irritation H361: Suspected of damaging fertility or the unborn child H373: May causes damage to organs through prolonged or repeated exposure H411: Toxic to aquatic life with long lasting effects
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. P264+P265: Wash hands thoroughly after handling. Do not touch eyes. P270: Do not eat, drink or smoke when using this product. P273: Avoid release to the environment. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
Response	P301+P317: IF SWALLOWED: Get medical help. P305+P351: IF IN EYES: Rinse cautiously with water for several minutes. P318: if exposed or concerned, get medical advice. P319: Get medical help if you feel unwell. P330: Rinse mouth. P337+P317: If eye irritation persists: Get medical help. P338: Remove contact lenses, if present and easy to do. Continue rinsing. P391: Collect spillage.
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: Myclobutanil

CAS Number: 88671-89-0

PubChem CID: 6336

Molecular formula: C15H17ClN4

Molecular weight: 288.77 g/mol

IUPAC name: 2-(4-chlorophenyl)-2-(1,2,4-triazol-1-ylmethyl)hexanenitrile

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Move to fresh air. Keep at rest in a position comfortable for breathing. Seek medical attention if symptoms persist.

Skin contact: Wash with plenty of soap and water. Remove contaminated clothing. Seek medical attention if irritation develops.

Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention.

Ingestion: Rinse mouth. Do NOT induce vomiting unless directed by medical personnel. Seek medical attention.

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

Excerpt from ERG Guide 151 [Substances - Toxic (Non-Combustible)]:

SMALL FIRE: Dry chemical, CO2 or water spray.

LARGE FIRE: Water spray, fog or regular foam. If it can be done safely, move undamaged containers away from the area around the fire. Dike runoff from fire control for later disposal. Avoid aiming straight or solid streams directly onto the product.

FIRE INVOLVING TANKS, RAIL TANK CARS OR HIGHWAY TANKS: Fight fire from maximum distance or use unmanned master stream devices 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 in direct contact with flames. For massive fire, use unmanned master stream devices or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2024)

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

Excerpt from ERG Guide 151 [Substances - Toxic (Non-Combustible)]:

IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.

SPILL: Increase the immediate precautionary measure distance, in the downwind direction, as necessary.

FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

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.

Do not discharge effluent containing this product into lakes, streams, ponds, estuaries, occans or other waters unless in accordance with the requirements of a National Pollutant Discharge Elimination System (NPDES) permit and the permitting authority has been notified in writing prior to dischape. Do not discharge effluent containing this product to sewer systems without previously notifying the local sewage treatment plant authority. For guidance contact your State Water Board or Regional Office of the EPA. /RH-3866 Technical/

Do not apply directly to water. Do not contaminate water when disposing of equipment washwaters. /Chemsico Fungicide Concentrate M6/

Do not contaminate water, food, or feed by ... disposal. ... Pesticide Disposal: Securely wrap original container in several layers of newspaper and discard in trash. Container DIsposal: Do not reuse container. Rinse thoroughly before discarding in trash. /Chemsico Fungicide Concentrate M6/

SRP: The scientific literature for the use of contact lenses in industry is conflicting. The benefit or detrimental effects of wearing contact lenses depend not only upon the substance, but also on factors including the form of the substance, characteristics and duration of the exposure, the uses of other eye protection equipment, and the hygiene of the lenses. However, there may be individual substances whose irritating or corrosive properties are such that the wearing of contact lenses would be harmful to the eye. In those specific cases, contact lenses should not be worn. In any event, the usual eye protection equipment should be worn even when contact lenses are in place. /Technical concentrates/

WARNING: Causes substantial but temporary eye injury. Do not get in eyes or on clothing. Wear protective eyewear (goggles, face shield, or safety glasses). Remove contaminated clothing and wash clothing before reuse. Harmful if swallowed. Wash thoroughly with soap and water after handling. /Chemsico Fungicide Concentrate M6/

Avoid contact with skin, eyes or clothing. Wear protective eyewear (goggles, face shield, or safety glasses). Remove contaminated clothing and wash clothing before reuse. Prolonged or frequently repeated skin contact may cause allergic reactions In some individuals. /RH-3866 Technical/

First Aid. If In Eyes: Hold eye open and rinse slowly and gently with water for 15 - 20 minutes. Remove contact lenses, If present, after the first 5 minutes, then continue rinsing eye. Call a Poison Control Center or doctor for treatment advice. If Swallowed: Call a Poison Control Center or doctor immediately for treatment advice. Have person sip a glass of water if able to swallow. Do not induce vomiting unless told to by a Poison Control Center or doctor. Do not give anything by mouth to an unconscious person. Have the product container or label with you when calling the Poison Control Center or doctor, or going for treatment. /Chemsico Fungicide Concentrate M6/

First Aid. If in eyes: Hold eye open and rinse slowly and gently with water for 15-20 minutes. Remove contact lenses, if present, after the first 5 minutes, then continue rinsing eye. Call a poison control center or doctor for treatment advice. If on skin or clothing: Take off contaminated clothing. Rinse skin immediately with plenty of water for 15-20 minutes. Call a poison control center or doctor for treatment advice. If swallowed: Call a poison control center or doctor immediately for treatment advice. Have a person sip a glass of water if able to swallow. Do not induce vomiting unless told to do so by a poison control center or doctor. Do not give anything by mouth to an unconscious person. If inhaled: Move person to fresh air. If person is not breathing, call 911 or an ambulance, then give artificial respiration ... Call a poison control center or doctor for further treatment advice. /RH-3866 Technical/

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Excerpt from ERG Guide 151 [Substances - Toxic (Non-Combustible)]:

Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Stop leak if you can do it without risk. Prevent entry into waterways, sewers, basements or confined areas. Cover with plastic sheet to prevent spreading. Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers. DO NOT GET WATER INSIDE CONTAINERS. For solids, prevent dust cloud and avoid inhalation of dust. (ERG, 2024)

Do not contaminate water, food, or feed by ... disposal. PesticIde Storage: Store in cool, dry area away from heat or open flame. /Chemsico Fungicide Concentrate M6/

7.2 Conditions for safe storage, including any incompatibilities

Do not contaminate water, food, or feed by ... disposal. PesticIde Storage: Store in cool, dry area away from heat or open flame. /Chemsico Fungicide Concentrate M6/

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 chemical safety goggles.

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: Myclobutanil is a light yellow solid used as a fungicide.

b) Odor: No data available

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: 63 to 68 °C

f) Initial boiling point and boiling range: 202 to 208 °C at 1 mm Hg

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: 0.0000016 [mmHg]

l) Vapor density: No data available

m) Relative density: No data available

n) Water solubility: Soluble in common organic solvents, e.g. ketones, esters, alcohols and aromatic hydrocarbons, all 50 to 100 g/L. Insoluble in aliphatic hydrocarbons.

o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 2.9

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): 54.5 Å²

Complexity: 345

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

Strong oxidizing agents, strong acids, strong bases.

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO□), Nitrogen oxides (NOx), Hydrogen chloride (HCl).

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

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

Oral Acute Reference Dose (RfDoa)(mg/kg-day): 0.6

Oral Acute Reference Dose Reference: OPP

Acute or One Day PAD (RfD) [mg/kg/day]: 0.6

Acute or One Day HHBPs [ppb]: 20000

Acute HHBP Sensitive Lifestage/Population: Females 13-49 yrs

Skin corrosion/irritation:

No data available.

Serious eye damage/eye irritation:

Causes serious eye irritation (H319).

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

No data available.

Carcinogenicity:

No data available.

Reproductive toxicity:

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

Specific target organ toxicity (single exposure):

H373

Specific target organ toxicity (repeated exposure):

No data available.

Aspiration hazard:

No data available.

11.2 Additional information

Carcinogen classification:

No indication of carcinogenicity to humans (not listed by IARC).

Signs and symptoms of exposure:

Workers exposed to myclobutanil have reported symptoms such as skin rash, allergic dermatitis, itchiness, nausea, heachache, diarrhea, abdominal pain, vomiting, nosebleed, and eye irritation (L2093).

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

LC50; Species: Lepomis macrochirus (Bluegill); Conditions: freshwater, static; Concentration: 2400 ug/L for 96 hr (95% confidence interval: 1500-4700 ug/L) /84.5% purity/

LC50; Species: Oncorhynchus mykiss (Rainbow trout); Conditions: freshwater, static; Concentration: 4200 ug/L for 96 hr (95% confidence interval: 3500-5600 ug/L) /84.5% purity/

LD50 /Colinus virginianus/ (Bobwhite quail) oral 510 mg/kg

LD50 Grey partridge oral 1635 mg/kg

For more Ecotoxicity Values (Complete) data for MYCLOBUTANIL (11 total), please visit the HSDB record page.

1.60e+03

2.10e+04

4.50e+02

4.0E+03(G)

5.60e+00

2.50e-02

Volatile

Mutagen

1

0.1

4.70e+03

6.20e+04

1.40e+03

4.0E+03 (G)

2.50e-02

Volatile

Mutagen

1

0.1

Myclobutanil's production may result in its release to the environment through various waste streams ; its use as a systemic fungicide will result in its direct release to the environment. If released to air, a vapor pressure of 1.6X10-6 mm Hg at 25 °C indicates myclobutanil will exist in both the vapor and particulate phases. Vapor-phase myclobutanil will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 2.3 days. Particulate-phase myclobutanil will be removed from the atmosphere by wet or dry deposition. Aqueous solutions of myclobutanil are decomposed by light with half-lives ranging from 25-222 days. Therefore, myclobutanil may be susceptible to direct photolysis in the atmosphere. If rel

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 2.9

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

This substance is classified as hazardous to the aquatic environment.

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).

DOT label: Poison

14.4 Packing group

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

14.5 Environmental hazards

Marine pollutant: Yes (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: Registered (REACH Active)

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

Environmental 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 - Developmental Toxicity; Reproductive Toxicity Authoritative List - Prop 65 Report - regardless of intended function of ingredient in the product

- EFSA Legal Basis: Commission Regulation (EC) No 1490/2002

- Safe Drinking Water Act: Myclobutanil is listed in the dataset of EPA Human Health Benchmarks for Pesticides under the Safe Drinking Water Act (40 eCFR 141)

- Status Regulation (EC): 2011/2/EU, Reg. (EU) 2018/155, Reg. (EU) 2022/801, Reg. (EU) No 540/2011

- FIFRA Requirements: Tolerances are established for combined residues of the fungicide myclobutanil alpha-butyl-alpha-(4-chlorophenyl)-1 H -1,2,4-triazole-1-propanenitrile and its alcohol metabolite (alpha-(3-hydroxybutyl)-alpha-(4-chlorophenyl)-1 H -1,2,4-triazole-1-propanenitrile (free and bound), in or on the followi

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: 2026/09/09

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.