

Celecoxib (SC-58635) SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- * Product Name: Celecoxib (SC-58635)
- * Catalog Number: S1261
- * CAS Number: 169590-42-5
- * IUPAC Name: 4-(5-p-tolyl-3-(trifluoromethyl)-1H-pyrazol-1-yl)benzenesulfonamide

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):

- Skin sensitization: Category 1. H317
- Serious eye irritation: Category 2. H319
- Reproductive toxicity: Category 1. H360
- Acute aquatic toxicity: Category 2. H401
- Chronic aquatic toxicity: Category 2. H411

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)

- H317: May cause an allergic skin reaction
- H319: Causes serious eye irritation
- H360: May damage fertility or the unborn child
- H401: Toxic to aquatic life
- H411: Toxic to aquatic life with long lasting effects

Precautionary statement(s)

None.

Prevention	P203: Obtain, read and follow all safety instructions before use. P261: Avoid breathing dust/fume/gas/mist/vapors/spray. P264+P265: Wash hands thoroughly after handling. Do not touch eyes. P272: Contaminated work clothing should not be allowed out of the workplace. P273: Avoid release to the environment. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
Response	P302+P352: IF ON SKIN: wash with plenty of water. P305+P351: IF IN EYES: Rinse cautiously with water for several minutes. P318: if exposed or concerned, get medical advice. P321: Specific treatment (see information on this label and safety datasheet)). P333+P317: If skin irritation or rash occurs: Get medical help. P337+P317: If eye irritation persists: Get medical help. P338: Remove contact lenses, if present and easy to do. Continue rinsing. P362+P364: Take off contaminated clothing and wash it before reuse. 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: Celecoxib (SC-58635)

CAS Number: 169590-42-5

PubChem CID: 2662

Molecular formula: C₁₇H₁₄F₃N₃O₂S

Molecular weight: 381.4 g/mol

IUPAC name: 4-[5-(4-methylphenyl)-3-(trifluoromethyl)pyrazol-1-yl]benzenesulfonamide

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

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Advice for firefighters: Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous decomposition products formed under fire conditions: Carbon oxides, Nitrogen oxides (NO_x), Sulfur oxides, Hydrogen fluoride.

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

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided. Methods and materials for containment and cleaning up: Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

SRP: Expired or waste pharmaceuticals shall carefully take into consideration applicable DEA, EPA, and FDA regulations. It is not appropriate to dispose by flushing the pharmaceutical down the toilet or discarding to trash. If possible return the pharmaceutical to the manufacturer for proper disposal being careful to properly label and securely package the material. Alternatively, the waste pharmaceutical shall be labeled, securely packaged and transported by a state licensed medical waste contractor to dispose by burial in a licensed hazardous or toxic waste landfill or incinerator.

Product: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Contaminated packaging: Dispose of as unused product.

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided. Precautions for safe handling: Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed.

Appropriate engineering controls: Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

SRP: Local exhaust ventilation should be applied wherever there is an incidence of point source emissions or dispersion of regulated contaminants in the work area. Ventilation control of the contaminant as close to its point of generation is both the most economical and safest method to minimize personnel exposure to airborne contaminants. Ensure that the local ventilation moves the contaminant away from the worker.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Keep container tightly closed in a dry and well-ventilated place.

Store at room temperature 20 °C to 25 °C (68 °F to 77 °F); excursions permitted between 15 °C to 30 °C (59 °F to 86 °F).

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Store at room temperature 20 °C to 25 °C (68 °F to 77 °F); excursions permitted between 15 °C to 30 °C (59 °F to 86 °F).

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: Solid
- b) Odor: No data available
- c) Odor threshold: No data available
- d) pH: No data available
- e) Melting point/freezing point: 157-159
- f) Initial boiling point and boiling range: 529.0±60.0
- 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: Poorly soluble
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 3.4
- 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): 86.4 Å²

Complexity: 577

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 (CO₂), Nitrogen oxides (NO_x), Sulfur oxides (SO_x), Hydrogen fluoride (HF).

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:

Causes serious eye irritation (H319).

Respiratory or skin sensitization:

May cause an allergic skin reaction (H317).

Germ cell mutagenicity:

No data available.

Carcinogenicity:

No data available.

Reproductive toxicity:

May damage fertility or the unborn child (H360).

Specific target organ toxicity (single exposure):

No data available.

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).

Exposure routes:

Well absorbed in the gastrointestinal tract. When a single dose of 200 mg is given to healthy subjects, peak plasma levels occur 3 hours after an oral dose. The peak plasma level is 705 ng/mL. Absolute bioavailability studies have not been conducted. When multiple doses are given, steady-state is reached on or before Day 5. When taken with a high fat meal, peak plasma levels are delayed for about 1 to 2 hours with an increase in total absorption (AUC) of 10% to 20%.

Signs and symptoms of exposure:

Symptoms of overdose include breathing difficulties, coma, drowsiness, gastrointestinal bleeding, high blood pressure, kidney failure, nausea, sluggishness, stomach pain, and vomiting.

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

EC50; Species: Ceriodaphnia dubia (Water Flea) age <24 hr; Conditions: freshwater, renewal, pH 7.6-8.8, dissolved oxygen 6.8-9.5 mg/L; Concentration: >1600 ug/L for 7 days; Effect: intoxication, immobilization />98% purity/

EC50; Species: Daphnia magna (Water Flea) age <24 hr; Conditions: freshwater, renewal, pH 7.6-8.8, dissolved oxygen 6.8-9.5 mg/L; Concentration: >890 ug/L for 7 days; Effect: intoxication, immobilization />98% purity/

Celecoxib's production and administration as a medication may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of 1.2×10^{-9} mm Hg at 25 °C indicates celecoxib will exist solely in the particulate phase in the ambient atmosphere. Particulate-phase celecoxib will be removed from the atmosphere by wet and dry deposition. Celecoxib contains chromophores that absorb at wavelengths >290 nm and, therefore, may be susceptible to direct photolysis by sunlight. If released to soil, celecoxib is expected to be immobile based upon an estimated Koc of 9.7×10^4 . Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 7.8×10^{-13} atm-cu m/mole. Volatilization from dry soil is not expected base upon its vapor pressure. Biodegradation data in soil or water were not available. If released into water, celecoxib is expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from w

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 3.4

Potential for bioaccumulation exists (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).

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: 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

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:

- FDA Requirements: The Approved Drug Products with Therapeutic Equivalence Evaluations identifies currently marketed prescription drug products, including celecoxib, approved on the basis of safety and effectiveness by FDA under sections 505 of the Federal Food, Drug, and Cosmetic Act.

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.