

CP21R7 SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: CP21R7

* Catalog Number: S7954

* CAS Number: 125314-13-8

* IUPAC Name: 1H-Pyrrole-2,5-dione, 3-(3-aminophenyl)-4-(1-methyl-1H-indol-3-yl)-

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):

Not classified as a hazardous substance according to GHS.

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s) None.

Signal Word Not applicable

Hazard statement(s) None.

Precautionary statement(s) None.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: CP21R7

CAS Number: 125314-13-8

PubChem CID: 5327711

Molecular formula: C₁₉H₁₅N₃O₂

Molecular weight: 317.3 g/mol

IUPAC name: 3-(3-aminophenyl)-4-(1-methylindol-3-yl)pyrrole-2,5-dione

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: breathing:

-- DO NOT perform mouth-to-mouth resuscitation; the victim may have ingested or inhaled the substance.

-- If equipped and pulse detected, wash face and mouth, then give artificial respiration using a proper respiratory medical device (bag-valve mask, pocket mask equipped with a one-way valve or other device).

-- If no pulse detected or no respiratory medical device available, provide continuous compressions. Conduct a pulse check every two minutes or monitor for any signs of spontaneous

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 135 [Substances - Spontaneously Combustible]:

DO NOT USE WATER, CO₂ OR FOAM ON MATERIAL ITSELF. Some of these materials may react violently with water. CAUTION: For Xanthates, UN3342 and for Dithionite (Hydrosulfite/Hydrosulphite) UN1384, UN1923 and UN1929, USE FLOODING AMOUNTS OF WATER for SMALL AND LARGE fires to stop the reaction. Smothering will not work for these materials, they do not need air to burn.

SMALL FIRE: Dry chemical, soda ash, lime or DRY sand, EXCEPT for UN1384, UN1923, UN1929 and UN3342.

LARGE FIRE: DRY sand, dry chemical, soda ash or lime EXCEPT for UN1384, UN1923, UN1929 and UN3342, or withdraw from area and let fire burn. CAUTION: UN3342 when flooded with water will continue to evolve flammable Carbon disulfide/Carbon disulphide vapors. If it can be done safely, move undamaged containers away from the area around the fire.

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 or in contact with substance. 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. (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

- CALL 911. Then call emergency response telephone number on shipping paper. If shipping paper not available or no answer, refer to appropriate telephone number listed on the inside back cover.

- Stay upwind, uphill and/or upstream.

- Keep unauthorized personnel away.

- ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area.

- Do not touch or walk through spilled material.

- Stop leak if you can do it without risk.

Small Spill

CAUTION: For spills of Xanthates, UN3342 and for Dithionite (Hydrosulfite/Hydrosulphite), UN1384, UN1923 and UN1929, dissolve in 5 parts water and collect for proper disposal.

CAUTION: UN3342 when flooded with water will continue to evolve flammable Carbon disulfide/Carbon disulphide vapors.

- Cover with DRY earth, DRY sand or other non-combustible material followed with plastic sheet to minimize spreading or contact with rain.

- Use clean, non-sparking tools to collect material and place it into loosely covered plastic containers for later disposal.

- Prevent entry into waterways, sewers, basements or confined areas.

- CALL 911. Then call emergency response telephone number on shipping paper. If shipping paper not available or no answer, refer to appropriate telephone number listed on the inside back cover.

- Stay upwind, uphill and/or upstream.

- Keep unauthorized personnel away.

- ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area.

- Do not touch or walk through spilled material.

- Stop leak if you can do it without risk.

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- Cover with DRY earth, DRY sand or other non-combustible material followed with plastic sheet to minimize spreading or contact with rain.
- Use clean, non-sparking tools to collect material and place it into loosely covered plastic containers for later disposal.
- Prevent entry into waterways, sewers, basements or confined areas.

Excerpt from ERG Guide 135 [Substances - Spontaneously 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)

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

- For highlighted materials: see Table 1 - Initial Isolation and Protective Action Distances.
- For non-highlighted materials: 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.

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

- For highlighted materials: see Table 1 - Initial Isolation and Protective Action Distances.
- For non-highlighted materials: 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.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Excerpt from ERG Guide 135 [Substances - Spontaneously Combustible]:

ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area. Do not touch or walk through spilled material. Stop leak if you can do it without risk.

SMALL SPILL: CAUTION: For spills of Xanthates, UN3342 and for Dithionite (Hydrosulfite/Hydrosulphite), UN1384, UN1923 and UN1929, dissolve in 5 parts water and collect for proper disposal. CAUTION: UN3342 when flooded with water will continue to evolve flammable Carbon disulfide/Carbon disulphide vapors. Cover with DRY earth, DRY sand or other non-combustible material followed with plastic sheet to minimize spreading or contact with rain. Use clean, non-sparking tools to collect material and place it into loosely covered plastic containers for later disposal. Prevent entry into waterways, sewers, basements or confined areas. (ERG, 2024)

7.2 Conditions for safe storage, including any incompatibilities

Store in a cool, dry, well-ventilated area. Keep container tightly closed.

Store away from incompatible materials (see Section 10).

Protect from light and moisture.

Recommended storage (industry convention for research compounds): -20°C for long-term storage; 2-8°C for short-term use and transport.

[Note: This is a general industry recommendation. Always verify exact storage conditions with the supplier Certificate of Analysis (COA).]

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: Product from the iron-oxide process for the removal of sulfides from gases. In this process gases are passed over a mixture of iron(III) oxide and wood shavings. Liable to spontaneous heating. This heat may cause ignition. Easily ignited by sparks or heat from external sources. Used for precipitating copper or lead from solutions of their salts and in electric furnace steel operations.

b) Odor: No data available

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: No data available

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: Soluble in DMSO; slightly soluble in water
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 2
- 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): 77.1 Å²

Complexity: 585

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).

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:

No data available.

Reproductive toxicity:

No data available.

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

No additional toxicological information available.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

No ecotoxicity data available.

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 2

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

UN 1376

14.2 UN proper shipping name

Consult official transport regulations (DOT/IATA/IMDG) for proper shipping name.

14.3 Transport hazard class(es)

Consult official transport regulations (DOT/IATA/IMDG) for hazard classification.

DOT label: Spontaneously Combustible

14.4 Packing group

Consult official transport regulations (DOT/IATA/IMDG) for packing group assignment.

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).

DOT Emergency Response Guide (ERG) number: 135

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: Not available in public databases.

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:

No SARA Hazards.

Massachusetts Right To Know Components:

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components:

No components are subject to the Pennsylvania Right to Know Act.

New Jersey Right To Know Components:

No components are subject to the New Jersey Right to Know Act.

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.

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: 2026/09/10

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.