1 Identification

· Product identifier
· Trade name: TMC-207
· Synonym
  (αS,βR)-6-bromo-α-[2-(dimethylamino)ethyl]-2-methoxy-α-1-naphthalenyl-β-phenyl-3-quinolineethanol
  Bedaquiline
  R207910
· Article number: 20247
· CAS Number: 843663-66-1
· EC number: 831-215-5
· Application of the substance / the mixture For research use only, not for human or veterinary use.
· Details of the supplier of the safety data sheet
  Manufacturer/Supplier:
  Cayman Chemical Co.
  1180 E. Ellsworth Rd.
  Ann Arbor, MI 48108
  USA
· Information department: Product safety department
· Emergency telephone number:
  During normal opening times: +1 (734) 971-3335
  US/CANADA: 800-424-9300
  Outside US/CANADA: 703-741-5970

2 Hazard(s) identification

· Classification of the substance or mixture
  GHS06 Skull and crossbones
  Acute Tox. 3 H301 Toxic if swallowed.
  GHS08 Health hazard
  STOT RE 2 H373 May cause damage to organs through prolonged or repeated exposure.
  GHS09 Environment
  Aquatic Acute 1 H400 Very toxic to aquatic life.
  Aquatic Chronic 1 H410 Very toxic to aquatic life with long lasting effects.
· Label elements
  GHS label elements
  The substance is classified and labeled according to the Globally Harmonized System (GHS).
Hazard pictograms

GHS06   GHS08   GHS09

Signal word Danger

Hazard statements
H301 Toxic if swallowed.
H373 May cause damage to organs through prolonged or repeated exposure.
H400 Very toxic to aquatic life.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements
Do not breathe dust/fume/gas/mist/vapors/spray.
Wash thoroughly after handling.
Do not eat, drink or smoke when using this product.
Avoid release to the environment.
If swallowed: Immediately call a poison center/doctor.
Specific treatment (see on this label).
Rinse mouth.
Get medical advice/attention if you feel unwell.
Collect spillage.
Store locked up.
Dispose of contents/container in accordance with local/regional/national/international regulations.

Classification system:

NFPA ratings (scale 0 - 4)

\[
\begin{array}{c|c|c}
 & Health & Fire & Reactivity \\
\hline
\text{Health} & 2 & 0 & 0 \\
\text{Fire} & 0 & 0 & 0 \\
\end{array}
\]

HMIS-ratings (scale 0 - 4)

\[
\begin{array}{c|c|c|c}
 & Health & Fire & Reactivity \\
\hline
\text{Health} & 2 & 0 & 0 \\
\text{Fire} & 0 & 0 & 0 \\
\end{array}
\]

Other hazards

Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances

CAS No. Description
843663-66-1 TMC-207

Identification number(s)
EC number: 831-215-5
4 First-aid measures

· Description of first aid measures
  · General information:
    Immediately remove any clothing soiled by the product.
    Symptoms of poisoning may even occur after several hours; therefore medical observation for at least
    48 hours after the accident.
    In case of irregular breathing or respiratory arrest provide artificial respiration.
  · After inhalation: In case of unconsciousness place patient stably in side position for transportation.
  · After skin contact: Immediately wash with water and soap and rinse thoroughly.
  · After eye contact: Rinse opened eye for several minutes under running water. Then consult a doctor.
  · After swallowing: Do not induce vomiting; immediately call for medical help.
  · Information for doctor:
    · Most important symptoms and effects, both acute and delayed
      May cause anemia, cough, CNS depression, drowsiness, headache, heart damage, lassitude
      (weakness, exhaustion), liver damage, narcosis, reproductive effects, teratogenic effects.
      No further relevant information available.
    · Indication of any immediate medical attention and special treatment needed
      No further relevant information available.

5 Fire-fighting measures

· Extinguishing media
· Suitable extinguishing agents:
  Use fire fighting measures that suit the environment.
  A solid water stream may be inefficient.
· Special hazards arising from the substance or mixture No further relevant information available.
· Advice for firefighters
· Protective equipment: No special measures required.

6 Accidental release measures

· Personal precautions, protective equipment and emergency procedures Not required.
· Environmental precautions:
  Inform respective authorities in case of seepage into water course or sewage system.
  Do not allow to enter sewers/ surface or ground water.
· Methods and material for containment and cleaning up:
  Dispose contaminated material as waste according to item 13.
· Reference to other sections
  See Section 7 for information on safe handling.
  See Section 8 for information on personal protection equipment.
  See Section 13 for disposal information.
· Protective Action Criteria for Chemicals
  · PAC-1: Substance is not listed.
  · PAC-2: Substance is not listed.
  · PAC-3: Substance is not listed.

7 Handling and storage

· Handling:
· Precautions for safe handling Thorough dedusting.
· Information about protection against explosions and fires: No special measures required.
· Conditions for safe storage, including any incompatibilities
· Storage:
· Requirements to be met by storerooms and receptacles: No special requirements.
· Information about storage in one common storage facility: Not required.
· Further information about storage conditions: None.
· Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

· Additional information about design of technical systems: No further data; see item 7.
· Control parameters
· Components with limit values that require monitoring at the workplace: Not required.
· Additional information: The lists that were valid during the creation were used as basis.
· Exposure controls
· Personal protective equipment:
· General protective and hygienic measures:
  Keep away from foodstuffs, beverages and feed.
  Immediately remove all soiled and contaminated clothing.
  Wash hands before breaks and at the end of work.
  Store protective clothing separately.
· Breathing equipment:
  In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.
· Protection of hands:

  Protective gloves

  The glove material has to be impermeable and resistant to the product/ the substance/ the preparation. Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture. Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation
· Material of gloves
  The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.
· Penetration time of glove material
  The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.
· Eye protection:

  Tightly sealed goggles
### 9 Physical and chemical properties

- **Information on basic physical and chemical properties**
  - **General Information**
  - **Appearance:**
    - Form: Crystalline
    - Color: Not determined.
  - **Odor:** Characteristic
  - **Structural Formula:** C$_{32}$H$_{31}$BrN$_2$O$_2$
  - **Molecular Weight:** 555.5 g/mol
  - **Odor threshold:** Not determined.
  - **pH-value:** Not applicable.
  - **Change in condition**
    - Melting point/Melting range: Undetermined.
    - Boiling point/Boiling range: Undetermined.
  - **Flash point:** Not applicable.
  - **Flammability (solid, gaseous):** Product is not flammable.
  - **Decomposition temperature:** Not determined.
  - **Auto igniting:** Not determined.
  - **Danger of explosion:** Product does not present an explosion hazard.
  - **Explosion limits:**
    - Lower: Not determined.
    - Upper: Not determined.
  - **Vapor pressure:** Not applicable.
  - **Density:** Not determined.
  - **Relative density:** Not determined.
  - **Vapor density:** Not applicable.
  - **Evaporation rate:** Not applicable.
  - **Solubility in / Miscibility with Water:** Not determined.
  - **Partition coefficient (n-octanol/water):** Not determined.
  - **Viscosity:**
    - Dynamic: Not applicable.
    - Kinematic: Not applicable.
  - **SOLUBILITY**
    - ~0.25 mg/ml in a 1:3 solution of DMF:PBS (pH 7.2): ~0.2,
    - 12.5, 25 mg/ml in EtOH, DMSO, DMF
  - **Other information**
    - No further relevant information available.

### 10 Stability and reactivity

- **Reactivity** No further relevant information available.
- **Chemical stability**
  - **Thermal decomposition / conditions to be avoided:**
    - No decomposition if used according to specifications.
  - **Possibility of hazardous reactions** No dangerous reactions known.
Safety Data Sheet  
acc. to OSHA HCS

Trade name: TMC-207

- Conditions to avoid: No further relevant information available.
- Incompatible materials: strong oxidizing agents
- Hazardous decomposition products: carbon oxides, hydrogen bromide, nitrogen oxides

11 Toxicological information

- RTECS Number VB8110000
- Information on toxicological effects
  - Acute toxicity:
    - Primary irritant effect:
      - on the skin: No irritant effect.
      - on the eye: No irritating effect.
  - Sensitization: No sensitizing effects known.
- Additional toxicological information:
  - Carcinogenic categories
    - IARC (International Agency for Research on Cancer) Substance is not listed.
    - NTP (National Toxicology Program) Substance is not listed.
    - OSHA-Ca (Occupational Safety & Health Administration) Substance is not listed.

12 Ecological information

- Toxicity
  - Aquatic toxicity: No further relevant information available.
  - Persistence and degradability No further relevant information available.
- Behavior in environmental systems:
  - Bioaccumulative potential No further relevant information available.
  - Mobility in soil No further relevant information available.
- Ecotoxicological effects:
  - Remark: Very toxic for fish
- Additional ecological information:
  - General notes:
    - Water hazard class 3 (Self-assessment): extremely hazardous for water
    - Do not allow product to reach ground water, water course or sewage system, even in small quantities.
    - Danger to drinking water if even extremely small quantities leak into the ground.
    - Also poisonous for fish and plankton in water bodies.
    - Very toxic for aquatic organisms
- Results of PBT and vPvB assessment
  - PBT: Not applicable.
  - vPvB: Not applicable.
- Other adverse effects No further relevant information available.

13 Disposal considerations

- Waste treatment methods
  - Recommendation:
    - Must not be disposed of together with household garbage. Do not allow product to reach sewage system.
Trade name: TMC-207

· Uncleaned packagings:
  · Recommendation: Disposal must be made according to official regulations.

## 14 Transport information

| · UN-Number                                      | UN2811 |
| · DOT, IMDG, IATA                                |        |

| · UN proper shipping name                        |
| · DOT                                           | Toxic solids, organic, n.o.s. (TMC-207) |
| · IMDG                                          | TOXIC SOLID, ORGANIC, N.O.S. (TMC-207) |
| · IATA                                          | Toxic solid, organic, n.o.s. (TMC-207) |

| · Transport hazard class(es)                     |
| · DOT                                           |
| · Class                                          | 6.1 Toxic substances |
| · Label                                          | 6.1 |

| · IMDG, IATA                                     |
| · Class                                          | 6.1 Toxic substances |
| · Label                                          | 6.1 |

| · Packing group                                  |
| · DOT, IMDG, IATA                                | III |

| · Environmental hazards:                         | Environmentally hazardous substance, solid |

| · Special precautions for user                   | Warning: Toxic substances |
| · Hazard identification number (Kemler code):     | 60 |
| · EMS Number:                                    | F-A,S-A |
| · Stowage Category                               | A |

| · Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code |
| · Not applicable. |

| · Transport/Additional information:              |
| · DOT                                           |
| · Quantity limitations                           |
| · On passenger aircraft/rail: 100 kg             |
| · On cargo aircraft only: 200 kg                 |

| · IMDG                                           |
| · Limited quantities (LQ)                        |
| · 5 kg                                           |
| · Code: E1                                       |

| · Excepted quantities (EQ)                       |
| · Maximum net quantity per inner packaging: 30 g |
| · Maximum net quantity per outer packaging: 1000 g |
Trade name: TMC-207

Remarks:
When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.

UN "Model Regulation":
UN 2811 TOXIC SOLID, ORGANIC, N.O.S. (TMC-207), 6.1, III, ENVIRONMENTALLY HAZARDOUS

15 Regulatory information

- Safety, health and environmental regulations/legislation specific for the substance or mixture
  No further relevant information available.
- Sara
- Section 355 (extremely hazardous substances): Substance is not listed.
- Section 313 (Specific toxic chemical listings): Substance is not listed.
- TSCA (Toxic Substances Control Act): Substance is not listed.
- Hazardous Air Pollutants Substance is not listed.
- Proposition 65
- Chemicals known to cause cancer: Substance is not listed.
- Chemicals known to cause reproductive toxicity for females: Substance is not listed.
- Chemicals known to cause reproductive toxicity for males: Substance is not listed.
- Chemicals known to cause developmental toxicity: Substance is not listed.
- Carcinogenic categories
- EPA (Environmental Protection Agency) Substance is not listed.
- TLV (Threshold Limit Value established by ACGIH) Substance is not listed.
- NIOSH-Ca (National Institute for Occupational Safety and Health) Substance is not listed.
- Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

- Department issuing SDS: Environment protection department.
- Contact: -
- Date of preparation / last revision 03/07/2021 / -
- Abbreviations and acronyms:
  IMDG: International Maritime Code for Dangerous Goods
  DOT: US Department of Transportation
  IATA: International Air Transport Association
  ACGIH: American Conference of Governmental Industrial Hygienists
  EINECS: European Inventory of Existing Commercial Chemical Substances
  CAS: Chemical Abstracts Service (division of the American Chemical Society)
  NFPA: National Fire Protection Association (USA)
  HMIS: Hazardous Materials Identification System (USA)
  PBT: Persistent, Bioaccumulative and Toxic
  vPvB: very Persistent and very Bioaccumulative
  NIOSH: National Institute for Occupational Safety
  OSHA: Occupational Safety & Health
  TLV: Threshold Limit Value
  PEL: Permissible Exposure Limit
  REL: Recommended Exposure Limit
<table>
<thead>
<tr>
<th>Trade name: TMC-207</th>
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<tbody>
<tr>
<td>Acute Tox. 3: Acute toxicity – Category 3</td>
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<tr>
<td>STOT RE 2: Specific target organ toxicity (repeated exposure) – Category 2</td>
</tr>
<tr>
<td>Aquatic Acute 1: Hazardous to the aquatic environment - acute aquatic hazard – Category 1</td>
</tr>
<tr>
<td>Aquatic Chronic 1: Hazardous to the aquatic environment - long-term aquatic hazard – Category 1</td>
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