

# Safety Data Sheet

acc. to OSHA HCS

Printing date 10/26/2020

Revision date 10/26/2020

## 1 Identification

- **Product identifier**
- **Trade name:** AB-FUBINACA metabolite 4
- **Synonym**  
1-[(4-fluorophenyl)methyl]-1H-indazole-3-carboxylic acid  
MMB-FUBINACA metabolite 4
- **Article number:** 20179
- **CAS Number:**  
50264-63-6
- **EC number:**  
696-501-2
- **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**



Acute Tox. 4 H302 Harmful if swallowed.

Acute Tox. 4 H312 Harmful in contact with skin.

Acute Tox. 4 H332 Harmful if inhaled.

- **Label elements**

- **GHS label elements**

The substance is classified and labeled according to the Globally Harmonized System (GHS).

- **Hazard pictograms**



- **Signal word** Warning

- **Hazard statements**

Harmful if swallowed, in contact with skin or if inhaled.

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- **Precautionary statements**

Avoid breathing dust/fume/gas/mist/vapors/spray  
 Wash thoroughly after handling.  
 Do not eat, drink or smoke when using this product.  
 Use only outdoors or in a well-ventilated area.  
 Wear protective gloves / protective clothing.  
 If swallowed: Call a poison center/doctor if you feel unwell.  
 If on skin: Wash with plenty of water.  
 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
 Specific treatment (see on this label).  
 Rinse mouth.  
 Take off contaminated clothing and wash it before reuse.  
 Dispose of contents/container in accordance with local/regional/national/international regulations.

- **Classification system:**

- **NFPA ratings (scale 0 - 4)**



Health = 3  
 Fire = 0  
 Reactivity = 0

- **HMIS-ratings (scale 0 - 4)**



Health = 2  
 Fire = 0  
 Reactivity = 0

- **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**  
50264-63-6 AB-FUBINACA metabolite 4
- **Identification number(s)**
- **EC number:** 696-501-2

## 4 First-aid measures

- **Description of first aid measures**
- **General information:**  
Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.
- **After inhalation:**  
Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.  
In case of unconsciousness place patient stably in side position for transportation.
- **After skin contact:** Generally the product does not irritate the skin.
- **After eye contact:** Rinse opened eye for several minutes under running water.
- **After swallowing:** Immediately call a doctor.

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- **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:** Mouth respiratory protective device.

## 6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures** Not required.
- **Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:** Ensure adequate ventilation.
- **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.  
Ensure good ventilation/exhaustion at the workplace.
- **Information about protection against explosions and fires:** No special measures required.
- **Conditions for safe storage, including any incompatibilities**  
Keep container tightly closed.  
Store in accordance with information listed on the product insert.
- **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:** Keep receptacle tightly sealed.
- **Specific end use(s)** No further relevant information available.

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## 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:**
  - The following constituent is the only constituent of the product which has a PEL, TLV or other recommended exposure limit.
  - The following constituents are the only constituents of the product which have a PEL, TLV or other recommended exposure limit.
  - At this time, the remaining constituent has no known exposure limits.
  - At this time, the other constituents have no known exposure limits.
- **Additional information:** The lists that were valid during the creation were used as basis.
- **Exposure controls**
- **Personal protective equipment:**
- **General protective and hygienic measures:**
  - Wash hands before breaks and at the end of work.
  - Avoid contact with the eyes and skin.
- **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:** Not required.

## 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<sub>15</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>2</sub>
- **Molecular Weight** 270.3 g/mol

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· <b>Odor threshold:</b>	Not determined.
· <b>pH-value:</b>	Not applicable.
· <b>Change in condition</b>	
<b>Melting point/Melting range:</b>	Undetermined.
<b>Boiling point/Boiling range:</b>	Undetermined.
· <b>Flash point:</b>	Not applicable.
· <b>Flammability (solid, gaseous):</b>	Product is not flammable.
· <b>Decomposition temperature:</b>	Not determined.
· <b>Auto igniting:</b>	Not determined.
· <b>Danger of explosion:</b>	Product does not present an explosion hazard.
· <b>Explosion limits:</b>	
<b>Lower:</b>	Not determined.
<b>Upper:</b>	Not determined.
· <b>Vapor pressure:</b>	Not applicable.
· <b>Density:</b>	Not determined.
· <b>Relative density</b>	Not determined.
· <b>Vapor density</b>	Not applicable.
· <b>Evaporation rate</b>	Not applicable.
· <b>Solubility in / Miscibility with Water:</b>	Not determined.
· <b>Partition coefficient (n-octanol/water):</b>	Not determined.
· <b>Viscosity:</b>	
<b>Dynamic:</b>	Not applicable.
<b>Kinematic:</b>	Not applicable.
· <b>Other information</b>	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.
- **Conditions to avoid** No further relevant information available.
- **Incompatible materials:** strong acids, strong bases, strong oxidizing agents, strong reducing agents
- **Hazardous decomposition products:** No dangerous decomposition products known.

## 11 Toxicological information

- **RTECS Number** NK7886400

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- **Information on toxicological effects**

- **Acute toxicity:**

- **LD/LC50 values that are relevant for classification:**

Oral	TDLO	377 mg/kg (rat)
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- **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.

- **Additional ecological information:**

- **General notes:**

Water hazard class 1 (Self-assessment): slightly hazardous for water

Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

- **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.

- **Uncleaned packagings:**

- **Recommendation:** Disposal must be made according to official regulations.

## 14 Transport information

- **UN-Number**

- **DOT, IMDG, IATA**

not regulated

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· <b>UN proper shipping name</b>	
· <b>DOT, IMDG, IATA</b>	not regulated
· <b>Transport hazard class(es)</b>	
· <b>DOT, ADN, IMDG, IATA</b>	
· <b>Class</b>	not regulated
· <b>Packing group</b>	
· <b>DOT, IMDG, IATA</b>	not regulated
· <b>Environmental hazards:</b>	Not applicable.
· <b>Special precautions for user</b>	Not applicable.
· <b>Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</b>	Not applicable.
· <b>UN "Model Regulation":</b>	not regulated

### 15 Regulatory information

- **Safety, health and environmental regulations/legislation specific for the substance or mixture**
- **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** 10/26/2020 / -

- **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)

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HMIS: Hazardous Materials Identification System (USA)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic

vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety &amp; Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

Acute Tox. 4: Acute toxicity – Category 4

**\* Data compared to the previous version altered.**

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