



Printing date 06/16/2020 Revision date 06/16/2020

1 Identification

· Product identifier

· Trade name: AB-CHMINACA metabolite M2

· Synonym N-[[1-(cyclohexylmethyl)-1H-indazol-3-yl]carbonyl]-L-valine

· Article number: 16389

· CAS Number: 1185887-51-7

· 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

The substance is not classified, according to the Globally Harmonized System (GHS).

- · Label elements
- · GHS label elements None
- · Hazard pictograms None
- · Signal word None
- · Hazard statements None
- · Classification system:
- · NFPA ratings (scale 0 4)



Health = 0Fire = 0Reactivity = 0

· HMIS-ratings (scale 0 - 4)



Health = 0 Fire = 0

Other hazards

· Results of PBT and vPvB assessment

· **PBT**: Not applicable.

· vPvB: Not applicable.

Printing date 06/16/2020 Revision date 06/16/2020

Trade name: AB-CHMINACA metabolite M2

(Contd. from page 1)

3 Composition/information on ingredients

· Chemical characterization: Substances

· CAS No. Description

1185887-51-7 AB-CHMINACA metabolite M2

4 First-aid measures

- · Description of first aid measures
- · General information: No special measures required.
- · After inhalation: Supply fresh air; consult doctor in case of complaints.
- 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: If symptoms persist consult doctor.
- 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: Do not allow to enter sewers/ surface or ground water.
- Methods and material for containment and cleaning up: Pick up mechanically.
- 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 No special measures required.

(Contd. on page 3)

Printing date 06/16/2020 Revision date 06/16/2020

Trade name: AB-CHMINACA metabolite M2

(Contd. from page 2)

· 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: 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:

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:

The usual precautionary measures for handling chemicals should be followed.

- · Breathing equipment: Not required.
- · Protection of hands:

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 C20H27N3O3

(Contd. on page 4)

Printing date 06/16/2020 Revision date 06/16/2020

Trade name: AB-CHMINACA metabolite M2

	(Contd. from page
· Molecular Weight	357.5 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/wa	ater): Not determined.
· Viscosity:	
Dynamic:	Not applicable.
Kinematic:	Not applicable.
SOLUBILITY	~0.5 mg/ml in a 1:1 solution of DMF:PBS (pH 7.2); ~30 mg/r
Other information	in EtOH & DMSO; ~50 mg/ml in 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.
- · Conditions to avoid No further relevant information available.
- · Incompatible materials: No further relevant information available.
- · Hazardous decomposition products: No dangerous decomposition products known.

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Printing date 06/16/2020 Revision date 06/16/2020

Trade name: AB-CHMINACA metabolite M2

(Contd. from page 4)

11 Toxicological information

- · 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:

When used and handled according to specifications, the product does not have any harmful effects according to our experience and the information provided to us.

The substance is not subject to classification.

- · 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:** Smaller quantities can be disposed of with household waste.
- Uncleaned packagings:
- · **Recommendation:** Disposal must be made according to official regulations.

14 Transport information

- · UN-Number
- · DOT, IMDG, IATA

not regulated

(Contd. on page 6)

Printing date 06/16/2020 Revision date 06/16/2020

Trade name: AB-CHMINACA metabolite M2

		(Contd. from page
· UN proper shipping name · DOT, IMDG, IATA	not regulated	
· Transport hazard class(es)		
· DOT, ADN, IMDG, IATA · Class	not regulated	
· Packing group · DOT, IMDG, IATA	not regulated	
· Environmental hazards:	Not applicable.	
· Special precautions for user	Not applicable.	
Transport in bulk according to Anne MARPOL73/78 and the IBC Code	x II of Not applicable.	
· UN "Model Regulation":	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.
- · GHS label elements None
- · Hazard pictograms None
- · Signal word None
- · Hazard statements None
- · 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 06/16/2020 / -
- Abbreviations and acronyms:

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation IATA: International Air Transport Association

(Contd. on page 7)

Printing date 06/16/2020 Revision date 06/16/2020

Trade name: AB-CHMINACA metabolite M2

ACGIH: American Conference of Governmental Industrial Hygienists 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 (Contd. from page 6)