

Safety Data Sheet

acc. to OSHA HCS

Printing date 07/09/2020

Revision date 07/09/2020

1 Identification

- **Product identifier**
- **Trade name:** ANA-12
- **Synonym**
N-[2-[[[(hexahydro-2-oxo-1H-azepin-3-yl)amino]carbonyl]phenyl]-benzo[b]thiophene-2-carboxamide
- **Article number:** 14309
- **Application of the substance** For research use only - not for human or veterinary use.
- **CAS Number:**
219766-25-3
- **EC number:**
803-090-7
- **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**



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

- **Label elements**
- **GHS label elements**
The substance is classified and labeled according to the Globally Harmonized System (GHS).
- **Hazard pictograms**



GHS07

- **Signal word** Warning
- **Hazard statements**
Harmful if swallowed.
- **Precautionary statements**
Wash thoroughly after handling.
Do not eat, drink or smoke when using this product.
If swallowed: Call a poison center/doctor if you feel unwell.
Rinse mouth.

(Contd. on page 2)

Safety Data Sheet

acc. to OSHA HCS

Printing date 07/09/2020

Revision date 07/09/2020

Trade name: ANA-12

(Contd. from page 1)

Dispose of contents/container in accordance with local/regional/national/international regulations.

- **Classification system:**

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



Health = 2
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**
219766-25-3 ANA-12
- **Identification number(s)**
- **EC number:** 803-090-7

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; 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:** Immediately call a 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.

(Contd. on page 3)

Safety Data Sheet

acc. to OSHA HCS

Printing date 07/09/2020

Revision date 07/09/2020

Trade name: ANA-12

(Contd. from page 2)

- **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 precautions are necessary if used correctly.
Avoid breathing dust/fume/gas/mist/vapours/spray.
Avoid prolonged or repeated exposure.
Keep away from sources of ignition.
Take precautionary measures against static discharge.re.
- **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.

(Contd. on page 4)

Safety Data Sheet

acc. to OSHA HCS

Printing date 07/09/2020

Revision date 07/09/2020

Trade name: ANA-12

(Contd. from page 3)

- **Exposure controls**
- **Personal protective equipment:**
- **General protective and hygienic measures:** Wash hands before breaks and at the end of work.
- **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	C22H21N3O3S
Molecular Weight	407.5 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.

(Contd. on page 5)

Safety Data Sheet

acc. to OSHA HCS

Printing date 07/09/2020

Revision date 07/09/2020

Trade name: ANA-12

(Contd. from page 4)

- **Solubility in / Miscibility with Water:** Not determined.
- **Partition coefficient (n-octanol/water):** Not determined.
- **Viscosity:**
 - Dynamic:** Not applicable.
 - Kinematic:** Not applicable.
- **SOLUBILITY** ~5 mg/ml in 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.
- **Conditions to avoid** No further relevant information available.
- **Incompatible materials:** strong oxidizing agents

Hazardous decomposition products:

219766-25-3 ANA-12 carbon oxides, nitrogen oxides, sulfur oxides

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:**
- **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

(Contd. on page 6)

Safety Data Sheet

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Revision date 07/09/2020

Trade name: ANA-12

(Contd. from page 5)

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

- **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 Annex II of MARPOL73/78 and the IBC Code**

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.

(Contd. on page 7)

Safety Data Sheet

acc. to OSHA HCS

Printing date 07/09/2020

Revision date 07/09/2020

Trade name: ANA-12

(Contd. from page 6)

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



GHS07

- **Signal word** Warning
- **Hazard statements**
Harmful if swallowed.
- **Precautionary statements**
Wash thoroughly after handling.
Do not eat, drink or smoke when using this product.
If swallowed: Call a poison center/doctor if you feel unwell.
Rinse mouth.
Dispose of contents/container in accordance with local/regional/national/international regulations.
- **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** 07/09/2020 / -
- **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)
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
Acute Tox. 4: Acute toxicity – Category 4

US