

according to Regulation (EC) No. 1907/2006 as amended by (EC) No. 2015/830 and US OSHA HCS 2015

Section 1. Identification of the Substance/Mixture and of the Company/Undertaking

- 1.1 Product Code:** 26150
Product Name: AT-121
Synonyms: N-[2-[1,2-dihydro-1'-[cis-4-(1-methylethyl)cyclohexyl]-3-oxospiro[isoquinoline-4(3H),4'-piperidin]-2-yl]ethyl]-sulfamide;
- 1.2 Relevant identified uses of the substance or mixture and uses advised against:**
Relevant identified uses: For research use only, not for human or veterinary use.
- 1.3 Details of the Supplier of the Safety Data Sheet:**
Company Name: Cayman Chemical Company
 1180 E. Ellsworth Rd.
 Ann Arbor, MI 48108
Web site address: www.caymanchem.com
Information: Cayman Chemical Company +1 (734)971-3335
- 1.4 Emergency telephone number:**
Emergency Contact: CHEMTREC Within USA and Canada: +1 (800)424-9300
 CHEMTREC Outside USA and Canada: +1 (703)527-3887

Section 2. Hazards Identification

- 2.1 Classification of the Substance or Mixture:**
Acute Toxicity: Inhalation, Category 3
Acute Toxicity: Oral, Category 4
Skin Corrosion/Irritation, Category 2
Serious Eye Damage/Eye Irritation, Category 2
Carcinogenicity, Category 2
Toxic To Reproduction, Category 2
Specific Target Organ Toxicity (repeated exposure), Category 1

2.2 Label Elements:



GHS Signal Word: **Danger**

GHS Hazard Phrases:

- H302: Harmful if swallowed.
 H315: Causes skin irritation.
 H319: Causes serious eye irritation.
 H331: Toxic if inhaled.
 H351: Suspected of causing cancer.
 H361: Suspected of damaging fertility or the unborn child.
 H372: Causes damage to organs through prolonged or repeated exposure.

GHS Precaution Phrases:

- P201: Obtain special instructions before use.
- P202: Do not handle until all safety precautions have been read and understood.
- P260: Do not breathe {dust/fume/gas/mist/vapors/spray}.
- P264: Wash {hands} thoroughly after handling.
- P280: Wear {protective gloves/protective clothing/eye protection/face protection}.

GHS Response Phrases:

- P301+312: IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.
- P302+352: IF ON SKIN: Wash with plenty of soap and water.
- P304+340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
- P305+351+338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- P308+313: IF exposed or concerned: Get medical attention/advice.
- P311: Call a POISON CENTER or doctor/physician.
- P314: Get medical attention/advice if you feel unwell.
- P321: Specific treatment {see ... on this label}.
- P330: Rinse mouth.
- P332+313: If skin irritation occurs, get medical advice/attention.
- P337+313: If eye irritation persists, get medical advice/attention.
- P362+364: Take off contaminated clothing and wash it before reuse.

GHS Storage and Disposal Phrases:

Please refer to Section 7 for Storage and Section 13 for Disposal information.

- 2.3 Adverse Human Health** Causes serious eye irritation.
- Effects and Symptoms:** Causes skin irritation.
 Harmful if swallowed.
 Material may be irritating to the mucous membranes and upper respiratory tract.
 May be harmful by skin absorption.
 May cause damage to organs through prolonged or repeated exposure.
 May cause respiratory system irritation.
 Suspected of causing cancer.
 Suspected of damaging fertility or the unborn child.
 Toxic if inhaled.
 To the best of our knowledge, the toxicological properties have not been thoroughly investigated.

Section 3. Composition/Information on Ingredients

CAS # / RTECS #	Hazardous Components (Chemical Name)/ REACH Registration No.	Concentration	EC No./ EC Index No.	GHS Classification
2099681-31-7 NA	AT-121	1.0 %	NA NA	No data available.
67-66-3 FS9100000	Chloroform 01-2119486657-20	99.0 %	200-663-8 602-006-00-4	Acute Tox.(O) 4: H302 Acute Tox.(I) 3: H331 Eye Damage 2: H319 Skin Corr. 2: H315 Carcinogen 2: H351 Toxic Repro. 2: H361d STOT (RE) 1: H372

Section 4. First Aid Measures

- 4.1 Description of First Aid Measures:**
- In Case of Inhalation:** Remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel. Get immediate medical attention.
- In Case of Skin Contact:** Immediately wash skin with soap and plenty of water for at least 15 minutes. Remove contaminated clothing. Get medical attention if symptoms occur. Wash clothing before reuse.
- In Case of Eye Contact:** Hold eyelids apart and flush eyes with plenty of water for at least 15 minutes. Have eyes examined and tested by medical personnel.
- In Case of Ingestion:** Wash out mouth with water provided person is conscious. Never give anything by mouth to an unconscious person. Get medical attention. Do NOT induce vomiting unless directed to do so by medical personnel.
- 4.2 Important Symptoms and Effects, Both Acute and Delayed:** Exposure may cause: dizziness, drowsiness, gastrointestinal disturbances, headache, lassitude, nausea, and vomiting.

Section 5. Fire Fighting Measures

- 5.1 Suitable Extinguishing Media:** Use alcohol-resistant foam, carbon dioxide, water, or dry chemical spray.
Use water spray to cool fire-exposed containers.
- Unsuitable Extinguishing Media:** A solid water stream may be inefficient.
- 5.2 Flammable Properties and Hazards:** No data available.
No data available.
- Flash Pt:** No data.
- Explosive Limits:** LEL: No data. UEL: No data.
- Autoignition Pt:** No data.
- 5.3 Fire Fighting Instructions:** As in any fire, wear self-contained breathing apparatus pressure-demand (NIOSH approved or equivalent), and full protective gear to prevent contact with skin and eyes.

Section 6. Accidental Release Measures

- 6.1 Protective Precautions, Protective Equipment and Emergency Procedures:** Avoid breathing vapors and provide adequate ventilation. As conditions warrant, wear a NIOSH approved self-contained breathing apparatus, or respirator, and appropriate personal protection (rubber boots, safety goggles, and heavy rubber gloves).
- 6.2 Environmental Precautions:** Take steps to avoid release into the environment, if safe to do so.
- 6.3 Methods and Material For Containment and Cleaning Up:** Contain spill and collect, as appropriate. Transfer to a chemical waste container for disposal in accordance with local regulations.

Section 7. Handling and Storage

- 7.1 Precautions To Be Taken in Handling:** Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid prolonged or repeated exposure.
- 7.2 Precautions To Be Taken in Storing:** Keep container tightly closed. Store in accordance with information listed on the product insert.

Section 8. Exposure Controls/Personal Protection

8.1 Exposure Parameters:

CAS #	Chemical Name	Jurisdiction	Recommended Exposure Limits	Notations
67-66-3	Chloroform	ACGIH TLV	TLV: 10 ppm	
		Europe	TWA: 10 mg/m3 (2 ppm)	Skin Absorption
		France VL	TWA: 10 mg/m3 (2 ppm) STEL: 250 mg/m3 (50 ppm)	
		OSHA PELs	CEIL: 50 ppm	
		Britain EH40	TWA: 9.9 mg/m3 (2 ppm) STEL: ()	Skin Absorption

8.2 Exposure Controls:

8.2.1 Engineering Controls (Ventilation etc.): Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits.

8.2.2 Personal protection equipment:

Eye Protection: Safety glasses

Protective Gloves: Compatible chemical-resistant gloves

Other Protective Clothing: Lab coat

Respiratory Equipment (Specify Type): NIOSH approved respirator, as conditions warrant.

Work/Hygienic/Maintenance Practices: Do not take internally.

Facilities storing or utilizing this material should be equipped with an eyewash and a safety shower.

Wash thoroughly after handling.

No data available.

Section 9. Physical and Chemical Properties

9.1 Information on Basic Physical and Chemical Properties

Physical States: [] Gas [X] Liquid [] Solid

Appearance and Odor: A solution in chloroform

pH: No data.

Melting Point: No data.

Boiling Point: No data.

Flash Pt: No data.

Evaporation Rate: No data.

Flammability (solid, gas): No data available.

Explosive Limits: LEL: No data. UEL: No data.

Vapor Pressure (vs. Air or mm Hg): 160 MM_HG at 20.0 C

Vapor Density (vs. Air = 1): No data.

Specific Gravity (Water = 1): No data.

Solubility in Water: No data.

Octanol/Water Partition Coefficient: No data.

Autoignition Pt:	No data.		
Decomposition Temperature:	No data.		
Viscosity:	No data.		
9.2 Other Information			
Percent Volatile:	No data.		
Molecular Formula & Weight:	C24H38N4O3	430.6	

Section 10. Stability and Reactivity

10.1 Reactivity:	No data available.		
10.2 Stability:	Unstable []	Stable [X]	
10.3 Stability Note(s):	Stable if stored in accordance with information listed on the product insert.		
Polymerization:	Will occur []	Will not occur [X]	
10.4 Conditions To Avoid:	protect from air, light, and heat		
10.5 Incompatibility - Materials To Avoid:	aluminum lithium magnesium potassium sodium/sodium oxides strong bases strong oxidizing agents		
10.6 Hazardous Decomposition or Byproducts:	carbon dioxide carbon monoxide chlorine hydrogen chloride gas phosgene gas		

Section 11. Toxicological Information

11.1 Information on Toxicological Effects:	The toxicological effects of this product have not been thoroughly studied. Chloroform - Toxicity Data: Oral LD50 (rat): 300 mg/kg; Oral LD50 (mouse): 36 mg/kg; Skin LD50 (rabbit): > 20 gm/kg; Inhalation TCLO (human): 5,000 mg/m3 (7m); Inhalation LC50 (rat): 47,702 mg/m3 (4h); Chloroform - Irritation Data: Skin (rabbit):10 mg (24h) mild; Eye (rabbit): 20 mg (24h) moderate;		
Chronic Toxicological Effects:	Chloroform - Investigated as an agricultural chemical, drug, mutagen, primary irritant, reproductive effector and tumorigen. Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here. See actual entry in RTECS for complete information. Chloroform RTECS Number: FS9100000.		
Carcinogenicity/Other Information:	Chloroform - California Prop. 65 carcinogen. Chloroform - IARC category 2B; NTP Carcinogen - reasonably anticipated;		
Carcinogenicity:	NTP? No	IARC Monographs? Yes	OSHA Regulated? No

CAS #	Hazardous Components (Chemical Name)	NTP	IARC	ACGIH	OSHA
2099681-31-7	AT-121	n.a.	n.a.	n.a.	n.a.
67-66-3	Chloroform	Possible	2B	A3	n.a.

Section 12. Ecological Information

- 12.1 Toxicity:** Avoid release into the environment.
Runoff from fire control or dilution water may cause pollution.
- 12.2 Persistence and Degradability:** No data available.
- 12.3 Bioaccumulative Potential:** No data available.
- 12.4 Mobility in Soil:** No data available.
- 12.5 Results of PBT and vPvB assessment:** No data available.
- 12.6 Other adverse effects:** No data available.

Section 13. Disposal Considerations

- 13.1 Waste Disposal Method:** Dispose in accordance with local, state, and federal regulations.

Section 14. Transport Information

14.1 LAND TRANSPORT (US DOT):

DOT Proper Shipping Name: Chloroform Solution
DOT Hazard Class: 6.1 POISON
UN/NA Number: UN1888 **Packing Group:** III



14.1 LAND TRANSPORT (European ADR/RID):

ADR/RID Shipping Name: Chloroform Solution
UN Number: 1888 **Packing Group:** III
Hazard Class: 6.1 - POISON

14.3 AIR TRANSPORT (ICAO/IATA):

ICAO/IATA Shipping Name: Chloroform Solution
UN Number: 1888 **Packing Group:** III
Hazard Class: 6.1 - POISON **IATA Classification:** 6.1

Additional Transport Information: Transport in accordance with local, state, and federal regulations.
 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.

Section 15. Regulatory Information

EPA SARA (Superfund Amendments and Reauthorization Act of 1986) Lists

CAS #	Hazardous Components (Chemical Name)	S. 302 (EHS)	S. 304 RQ	S. 313 (TRI)
2099681-31-7	AT-121	No	No	No
67-66-3	Chloroform	Yes 10000 LB	Yes 10 LB	Yes

CAS #	Hazardous Components (Chemical Name)	Other US EPA or State Lists
2099681-31-7	AT-121	CAA HAP,ODC: No; CWA NPDES: No; TSCA: No; CA PROP.65: No
67-66-3	Chloroform	CAA HAP,ODC: HAP: VHAP; CWA NPDES: Yes; TSCA: Yes



SAFETY DATA SHEET

AT-121

	- Inventory, 8A CAIR; CA PROP.65: Yes: Canc+RDTox.
--	--

Regulatory Information Statement:	This SDS was prepared in accordance with 29 CFR 1910.1200 and Regulation (EC) No.1272/2008.
--	---

Section 16. Other Information

Revision Date: 07/12/2019

Additional Information About This Product: No data available.

Company Policy or Disclaimer: DISCLAIMER: This information is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes.