

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/21/2020

Revision date 09/21/2020

1 Identification

- **Product identifier**
- **Trade name:** **H3B-5942**
- **Synonym**
(2E)-4-[[2-[4-[(1E)-1-(1H-indazol-5-yl)-2-phenyl-1-buten-1-yl]phenoxy]ethyl]amino]-N,N-dimethyl-2-butenamide
- **Article number:** 31454
- **CAS Number:**
2052128-15-9
- **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.
Skin Irrit. 2 H315 Causes skin irritation.
Eye Irrit. 2A H319 Causes serious eye irritation.
STOT SE 3 H335 May cause respiratory irritation.

- **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.
Causes skin irritation.
Causes serious eye irritation.

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May cause respiratory irritation.

- **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 / eye protection / face protection.

If swallowed: Call a poison center/doctor if you feel unwell.

Rinse mouth.

If on skin: Wash with plenty of water.

Specific treatment (see on this label).

IF INHALED: Remove person to fresh air and keep comfortable for breathing.

If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

If skin irritation occurs: Get medical advice/attention.

Take off contaminated clothing and wash it before reuse.

If eye irritation persists: Get medical advice/attention.

Store in a well-ventilated place. Keep container tightly closed.

Store locked up.

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**

2052128-15-9 H3B-5942

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:** In case of unconsciousness place patient stably in side position for transportation.

- **After skin contact:** Immediately wash with water and soap and rinse thoroughly.

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- **After eye contact:**
Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.
- **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.
- **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:** 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**
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.

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- **Further information about storage conditions:** Keep receptacle tightly sealed.
- **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:**
 - Keep away from foodstuffs, beverages and feed.
 - Immediately remove all soiled and contaminated clothing.
 - 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:**



Tightly sealed goggles

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9 Physical and chemical properties

· Information on basic physical and chemical properties

· General Information

· Appearance:

Form: Crystalline
Color: Not determined.

· Odor: Characteristic

· Structural Formula: C₃₁H₃₄N₄O₂

· Molecular Weight: 494.6 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); ~5, 1, 30 mg/ml in EtOH, DMSO, DMF, respectively

· 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.

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- **Incompatible materials:** No further relevant information available.
- **Hazardous decomposition products:** carbon oxides, nitrogen oxides

11 Toxicological information

- **Information on toxicological effects**
- **Acute toxicity:**
- **Primary irritant effect:**
- **on the skin:** Irritant to skin and mucous membranes.
- **on the eye:** 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.

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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.
- **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.
Causes skin irritation.
Causes serious eye irritation.

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- May cause respiratory irritation.
- **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 / eye protection / face protection.
- If swallowed: Call a poison center/doctor if you feel unwell.
- Rinse mouth.
- If on skin: Wash with plenty of water.
- Specific treatment (see on this label).
- IF INHALED: Remove person to fresh air and keep comfortable for breathing.
- If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- If skin irritation occurs: Get medical advice/attention.
- Take off contaminated clothing and wash it before reuse.
- If eye irritation persists: Get medical advice/attention.
- Store in a well-ventilated place. Keep container tightly closed.
- Store locked up.
- 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** 09/21/2020 / -
- **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
- CAS: Chemical Abstracts Service (division of the American Chemical Society)
- NFPA: National Fire Protection Association (USA)
- HMS: 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
- Skin Irrit. 2: Skin corrosion/irritation – Category 2
- Eye Irrit. 2A: Serious eye damage/eye irritation – Category 2A
- STOT SE 3: Specific target organ toxicity (single exposure) – Category 3
- *** Data compared to the previous version altered.**

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