

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations SDS ID: 3H37B00 Issue date: 12/13/2022 Version: 1.0

| SECTION 1: Identification | |
|--|--|
| 1.1. Identification | |
| Product form Substance name CAS-No. Product code Formula Other means of identification | Substance 3-Bromo-1H-indole-2-carbonitrile 1373348-93-6 3H37-B-00 C9H5BrN2 MFCD22126115 |
| 1.2. Recommended use and restrictions o | n use |
| Use of the substance/mixture | : Laboratory chemicals Manufacture of substances Scientific research and development |
| 1.3. Supplier | |
| SynQuest Laboratories, Inc. Inc. P.O. Box 309 Alachua, FL, Alachua, 32615 United States of America T (386) 462-0788 - F (386) 462-7097 info@synquestlabs.com - www.synquestlabs.com | |
| 1.4. Emergency telephone number | |
| Emergency number | : (844) 523-4086 (3E Company - Account 10069) |
| SECTION 2: Hazard(s) identification | |
| 2.1. Classification of the substance or mix | cture |
| GHS US classification | |
| Acute toxicity (oral) Category 3 | H301 Toxic if swallowed H312 Harmful in contact with skin |

| Acute toxicity (oral) category 5 | 11501 | TOXIC II SWalloweu |
|---|-------|----------------------------------|
| Acute toxicity (dermal) Category 4 | H312 | Harmful in contact with skin |
| Acute toxicity (inhalation) Category 4 | H332 | Harmful if inhaled |
| Skin corrosion/irritation Category 2 | H315 | Causes skin irritation |
| Serious eye damage/eye irritation Category 2A | H319 | Causes serious eye irritation |
| Specific target organ toxicity – Single exposure, Category 3, | H335 | May cause respiratory irritation |
| Respiratory tract irritation | | |
| Full text of H statements : see section 16 | | |

2.2. GHS Label elements, including precautionary statements

GHS US labeling

Hazard pictograms (GHS US)

Signal word (GHS US) Hazard statements (GHS US)



: Danger

:

: H301 - Toxic if swallowed H312+H332 - Harmful in contact with skin or if inhaled H315 - Causes skin irritation

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| Precautionary statements (GHS US) | H319 - Causes serious eye irritation H335 - May cause respiratory irritation P261 - Avoid breathing dust, mist, spray. P264 - Wash skin thoroughly after handling P270 - Do not eat, drink or smoke when using this product. P271 - Use only outdoors or in a well-ventilated area. P280 - Wear protective gloves/protective clothing/eye protection/face protection. P301+P310 - If swallowed: Immediately call a poison center or doctor. P302+P352 - If on skin: Wash with plenty of soap and water P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing. P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove |
|-----------------------------------|--|
| | contact lenses, if present and easy to do. Continue rinsing. P312 - Call a POISON CENTER or doctor/physician if you feel unwell P321 - Specific treatment (see supplemental first aid instructions on this label) P322 - Specific treatment (see supplemental first aid instruction on this label) P330 - Rinse mouth. P332+P313 - If skin irritation occurs: Get medical advice/attention. P337+P313 - If eye irritation persists: Get medical advice/attention. P362+P364 - Take off contaminated clothing and wash it before reuse. P403+P233 - Store in a well-ventilated place. Keep container tightly closed. P405 - Store locked up. P501 - Dispose of contents/container to an approved waste disposal plant |

2.3. Other hazards which do not result in classification

No additional information available

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/Information on ingredients

3.1. Substances

Substance type

: Mono-constituent

| Name | Product identifier | % | GHS US classification |
|--|---------------------------|---|--|
| 3-Bromo-1H-indole-2-carbonitrile (Main constituent) | CAS-No.: 1373348- 93-6 | | Acute Tox. 3 (Oral), H301 Acute Tox. 4 (Dermal), H312 Acute Tox. 4 (Inhalation), H332 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335 |

Full text of hazard classes and H-statements : see section 16

3.2. Mixtures

Not applicable

| SECTION 4: First-aid measures | |
|--|--|
| 4.1. Description of first aid measures | |
| First-aid measures general | : In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Move the affected personnel away from the contaminated area. |

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| First-aid measures after inhalation | : Remove person to fresh air and keep comfortable for breathing. If not breathing, give artificial respiration. Get immediate medical advice/attention. |
|---------------------------------------|---|
| First-aid measures after skin contact | : Wash with plenty of soap and water. Get immediate medical advice/attention. |
| First-aid measures after eye contact | : Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get immediate medical advice/attention. |
| First-aid measures after ingestion | : Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get immediate medical advice/attention. |
| 4.2. Most important symptoms and effe | cts (acute and delayed) |
| Symptoms/effects | : The most important known symptoms and effects are described in the labelling (see section 2.2) |

and/or in section 11.

4.3. Immediate medical attention and special treatment, if necessary

Treat symptomatically.

| SECTION 5: Fire-fighting measures | | |
|---|---|--|
| 5.1. Suitable (and unsuitable) extinguishing | media | |
| Suitable extinguishing media | : Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media appropriate for surrounding fire. | |
| 5.2. Specific hazards arising from the chemical | | |
| Fire hazard | : Thermal decomposition generates: Carbon oxides. Hydrogen bromide. Hydrogen fluoride. Nitrogen oxides. | |
| 5.3. Special protective equipment and preca | autions for fire-fighters | |
| Firefighting instructions Protection during firefighting | In case of fire: Evacuate area. Wear gas tight chemically protective clothing in combination with self contained breathing apparatus. For further information refer to section 8: "Exposure controls/personal protection". | |

| SECTION 6: Accidental release measures | | | |
|--|---|--|--|
| 6.1. Personal precautions, protectiv | 6.1. Personal precautions, protective equipment and emergency procedures | | |
| General measures | : Evacuate unnecessary personnel. Ensure adequate air ventilation. Do not breathe dust. | | |
| 6.1.1. For non-emergency personnel | | | |
| Emergency procedures | : Only qualified personnel equipped with suitable protective equipment may intervene. | | |
| 6.1.2. For emergency responders | | | |
| Protective equipment | : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection". | | |
| 6.2. Environmental precautions | | | |

Avoid release to the environment. Notify authorities if product enters sewers or public waters.

| 6.3. Methods and material for contain | ment and cleaning up |
|---|---|
| For containment Methods for cleaning up Other information | Stop leak if safe to do so. Sweep or shovel spills into appropriate container for disposal. Minimize generation of dust. For disposal of solid materials or residues refer to section 13 : "Disposal considerations". |
| 6.4. Reference to other sections | |

No additional information available

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| SECTION 7: Handling and storage | | | |
|---|--|--|--|
| 7.1. Precautions for safe handling | | | |
| | Do not handle until all safety precautions have been read and understood. Ensure good ventilation of the work station. Do not breathe dust, mist, spray. Wear personal protective equipment. Avoid contact with skin and eyes. Handle in accordance with good industrial hygiene and safety procedures. Do not eat, drink or smoke when using this product. Always wash hands after handling the product. | | |
| 7.2. Conditions for safe storage, including an | ny incompatibilities | | |
| | Comply with applicable regulations. Keep container closed when not in use. Keep away from ignition sources. Air sensitive. Keep contents under inert gas. Refer to Section 10 on Incompatible Materials. Store in dry, cool, well-ventilated area. | | |
| SECTION 8: Exposure controls/personal | protection | | |
| 8.1. Control parameters | | | |
| 3-Bromo-1H-indole-2-carbonitrile (1373348-9 | 13-6) | | |
| No additional information available | | | |
| 8.2. Appropriate engineering controls | | | |
| Appropriate engineering controls | : Ensure good ventilation of the work station. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure. | | |
| 8.3. Individual protection measures/Personal | protective equipment | | |
| Hand protection: | | | |
| protective gloves. 29 CFR 1910.138: Hand Protection | 1 | | |
| Eye protection: | | | |
| Chemical goggles or safety glasses. Face shield. 29 CFR 1910.133: Eye and Face Protection | | | |
| Skin and body protection: | | | |
| Wear suitable protective clothing | | | |
| Respiratory protection: | | | |

In case of inadequate ventilation wear respiratory protection. 29 CFR 1910.134: Respiratory Protection

Personal protective equipment symbol(s):



Other information:

Safety shoes. 29 CFR 1910.136: Foot Protection.

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SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

| Physical state | : Solid |
|---|---------------------|
| Color | : No data available |
| Odor | : No data available |
| Odor threshold | : No data available |
| рН | : No data available |
| Melting point | : 176 – 178 °C |
| Freezing point | : No data available |
| Boiling point | : No data available |
| Flash point | : No data available |
| Relative evaporation rate (butyl acetate=1) | : No data available |
| Flammability (solid, gas) | : No data available |
| Vapor pressure | : No data available |
| Relative vapor density at 20 °C | : No data available |
| Relative density | : No data available |
| Molecular mass | : 221.053 g/mol |
| Solubility | : No data available |
| Partition coefficient n-octanol/water (Log Pow) | : No data available |
| Auto-ignition temperature | : No data available |
| Decomposition temperature | : No data available |
| Viscosity, kinematic | : No data available |
| Viscosity, dynamic | : No data available |
| Explosion limits | : No data available |
| Explosive properties | : No data available |
| Oxidizing properties | : No data available |
| | |

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

The product is stable at normal handling and storage conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Keep away from heat, sparks and flame.

10.5. Incompatible materials

Acids. Strong oxidizing agents.

10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced. Hazardous decomposition products in case of fire, see Section 5.

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SECTION 11: Toxicological information

| 11.1. Information on toxicological effe | ects |
|---|--|
| Acute toxicity (oral) | : Toxic if swallowed. |
| Acute toxicity (dermal) | : Harmful in contact with skin. |
| Acute toxicity (inhalation) | : Harmful if inhaled. |
| Skin corrosion/irritation | : Causes skin irritation. |
| Serious eye damage/irritation | : Causes serious eye irritation. |
| Respiratory or skin sensitization | : Not classified |
| Germ cell mutagenicity | : Not classified |
| Carcinogenicity | : Not classified |
| Reproductive toxicity | : Not classified |
| STOT-single exposure | : May cause respiratory irritation. |
| STOT-repeated exposure | : Not classified |
| Aspiration hazard | : Not classified |
| Viscosity, kinematic | : No data available |
| Symptoms/effects | : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11. |

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

No additional information available

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Disposal methods

Waste treatment methods Product/Packaging disposal recommendations Additional information

- Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.
 Dispose of contents/container in accordance with licensed collector's sorting instructions.
- : Recycle the material as far as possible.

| SECTION 14: Transport information | | |
|--|--|--|
| 14.1. UN number | | |
| DOT NA No UN-No. (TDG) UN-No. (IMDG) | : UN3439 : Not applicable : 3439 | |

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| UN-No. (IATA) | : 3439 |
|--|--|
| 14.2. UN proper shipping name Proper Shipping Name (DOT) Proper Shipping Name (TDG) Proper Shipping Name (IMDG) Proper Shipping Name (IATA) | Nitriles, solid, toxic, n.o.s. Not applicable NITRILES, SOLID, TOXIC, N.O.S. Nitriles, solid, toxic, n.o.s. |
| 14.3. Transport hazard class(es) | |
| DOT Transport hazard class(es) (DOT) Hazard labels (DOT) | : 6.1 : 6.1 |
| TDG Transport hazard class(es) (TDG) | : Not applicable |
| IMDG Transport hazard class(es) (IMDG) Hazard labels (IMDG) | : 6.1 : 6.1 |
| IATA Transport hazard class(es) (IATA) Hazard labels (IATA) | : 6.1 : 6.1 |
| 14.4. Packing group | |
| Packing group (DOT) Packing group (TDG) Packing group (IMDG) Packing group (IATA) | : III : Not applicable : III : III |
| 14.5. Environmental hazards | |
| Other information | : No supplementary information available. |
| 14.6. Special precautions for user | |
| DOT UN-No.(DOT) | : UN3439 |

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| DOT Special Provisions (49 CFR 172.102) | IB8 - Authorized IBCs: Metal (11A, 11B, 11N, 21A, 21B, 21N, 31A, 31B and 31N); Rigid plastics (11H1, 11H2, 21H1, 21H2, 31H1 and 31H2); Composite (11HZ1, 11HZ2, 21HZ1, 21HZ2, 31HZ1 and 31HZ2); Fiberboard (11G); Wooden (11C, 11D and 11F); Flexible (13H1, 13H2, 13H3, 13H4, 13H5, 13L1, 13L2, 13L3, 13L4, 13M1 or 13M2). IP3 - Flexible IBCs must be sift-proof and water-resistant or must be fitted with a sift-proof and water-resistant liner. T1 - 1.5 178.274(d)(2) Normal 178.275(d)(2) TP33 - The portable tank instruction assigned for this substance applies for granular and powdered solids and for solids which are filled and discharged at temperatures above their melting point which are cooled and transported as a solid mass. Solid substances transported or offered for transport above their melting point are authorized for transportation in portable tanks conforming to the provisions of portable tank instruction T4 for solid substances of packing group III or T7 for solid substances of packing group II, unless a tank with more stringent requirements for minimum shell thickness, maximum allowable working pressure, pressure-relief devices or bottom outlets are assigned in which case the more stringent tank instruction and special provisions shall apply. Filling limits must be in accordance with portable tank special provision |
|--|---|
| | accordance with the applicable requirements of this subchapter. |
| DOT Packaging Exceptions (49 CFR 173.xxx) | : 153 |
| DOT Packaging Non Bulk (49 CFR 173.xxx) | : 213 |
| DOT Packaging Bulk (49 CFR 173.xxx) | : 240 |
| DOT Quantity Limitations Passenger aircraft/rail (49 | : 100 kg |
| CFR 173.27) | |
| DOT Quantity Limitations Cargo aircraft only (49 | : 200 kg |
| CFR 175.75) | |
| DOT Vessel Stowage Location | : A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a |
| | passenger vessel. |
| DOT Vessel Stowage Other | : 52 - Stow "separated from" acids |
| TDG Emergency Response Guide (ERG) Number | : 151 |
| IMDG | |
| Special provision (IMDG) | : 223, 274 |
| Limited quantities (IMDG) | : 5 kg |
| Excepted quantities (IMDG) | : E1 |
| Packing instructions (IMDG) | : P002, LP02 |
| IBC packing instructions (IMDG) | : IBC08 |
| IBC special provisions (IMDG) | : B3 |
| Tank instructions (IMDG) | : T1 . TP22 |
| Tank special provisions (IMDG) EmS-No. (Fire) | : TP33 : F-A - FIRE SCHEDULE Alfa - GENERAL FIRE SCHEDULE |
| EmS-No. (Spillage) | : S-A - SPILLAGE SCHEDULE Alfa - TOXIC SUBSTANCES |
| | |
| Stowage category (IMDG) Segregation (IMDG) | : A : SG35 |
| Properties and observations (IMDG) | : Solid, evolving toxic vapours. Reacts with acids or acid fumes, evolving hydrogen cyanide, a |
| | highly toxic and flammable gas. Soluble in water. Toxic if swallowed, by skin contact or by inhalation. |
| ΙΑΤΑ | |
| PCA Excepted quantities (IATA) | : E1 |
| PCA Limited quantities (IATA) | : Y645 |
| PCA limited quantity max net quantity (IATA) | : 10kg |
| PCA packing instructions (IATA) | : 670 |
| PCA max net quantity (IATA) | : 100kg |
| CAO packing instructions (IATA) | : 677 |
| CAO max net quantity (IATA) | : 200kg |
| Special provision (IATA) | : A3, A5 |
| ERG code (IATA) | : 6L |
| | |

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14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

| SECTION 15: Regulatory information | | | |
|--|---|---|--|
| 15.1. US Federal regulations | | | |
| All components of this product are present and (TSCA) inventory, except for: | listed as Active on the United States Env | ironmental Protection Agency Toxic Substances Control Act | |
| 3-Bromo-1H-indole-2-carbonitrile | CAS-No. 1373348-93-6 | 100% | |
| 15.2. International regulations | | | |
| CANADA | | | |
| No additional information available | | | |
| EU-Regulations | | | |
| No additional information available | | | |
| National regulations | | | |
| No additional information available | | | |
| 15.3. US State regulations | | | |

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

SECTION 16: Other information

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| Full text of H-phrases | |
|------------------------|----------------------------------|
| H301 | Toxic if swallowed |
| H312 | Harmful in contact with skin |
| H315 | Causes skin irritation |
| H319 | Causes serious eye irritation |
| H332 | Harmful if inhaled |
| H335 | May cause respiratory irritation |

| NFPA health hazard | : 2 - Materials that, under emergency conditions, can cause temporary | |
|--------------------|--|--|
| NFPA fire hazard | incapacitation or residual injury. : 1 - Materials that must be preheated before ignition can occur. | |
| NFPA reactivity | : 0 - Material that in themselves are normally stable, even under fire conditions. | |
| Hazard Rating | | |
| Health | : 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given | |
| Flammability | : 1 Slight Hazard - Materials that must be preheated before ignition will occur. Includes liquids, solids and semi solids having a flash point above 200 F. (Class IIIB) | |

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Physical

: 0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

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