

# SAFETY DATA SHEET

according to the OSHA  
Hazard Communication Standard

Version 8.2  
Revision Date 05/18/2026  
Print Date 05/19/2026

## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : Amisulbrom Metabolite IT-14

Product Number : 94026  
Brand : Supelco

### 1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

### 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

### 1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week

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## SECTION 2. HAZARDS IDENTIFICATION

**GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)**

**Hazards for the product as supplied**

Acute toxicity (Oral) : Category 3

Reproductive toxicity : Category 2

Short-term (acute) aquatic hazard : Category 1

Long-term (chronic) aquatic hazard : Category 2

#### Other hazards

None known.

#### GHS label elements

Hazard pictograms :



Signal word : Danger

Hazard statements : H301 Toxic if swallowed.  
H361 Suspected of damaging fertility or the unborn child.  
H400 Very toxic to aquatic life.  
H411 Toxic to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**  
P201 Obtain special instructions before use.  
P202 Do not handle until all safety precautions have been read and understood.  
P264 Wash skin thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

**Response:**  
P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.  
P308 + P313 IF exposed or concerned: Get medical advice/ attention.  
P391 Collect spillage.

**Storage:**  
P405 Store locked up.

**Disposal:**  
P501 Dispose of contents/ container to an approved waste disposal plant.

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### SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

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Substance / Mixture : Substance  
CAS-No. : Not Assigned

### Components

| Chemical name                                                                    | CAS No./Unique ID | Concentration (% w/w) | Trade secret |
|----------------------------------------------------------------------------------|-------------------|-----------------------|--------------|
| 3-Bromo-6-fluoro-2-methyl-1-((1-methyl-1H-1,2,4-triazol-3-yl)sulfonyl)-1H-indole | -                 | $\geq 90 - \leq 100$  | -            |

Actual concentration is withheld as a trade secret

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## SECTION 4. FIRST AID MEASURES

General advice : Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air. Call in physician.

In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact : After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed : If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

Most important symptoms and effects, both acute and delayed : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

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## SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media : Water  
Foam

Carbon dioxide (CO<sub>2</sub>)  
Dry powder

Unsuitable extinguishing media : For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting : Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products : Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Sulphur oxides

Hydrogen bromide gas

Hydrogen fluoride

Specific extinguishing methods : No data available

Further information : Suppress (knock down) gases/vapours/mists with a water spray jet.  
Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:  
Avoid inhalation of dusts.  
Avoid substance contact.  
Ensure adequate ventilation.  
Evacuate the danger area, observe emergency

procedures, consult an expert.  
Advice for emergency responders:  
For personal protection see section 8.

|                                                       |                                                                                                                                                                                                                      |
|-------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Environmental precautions                             | : Do not let product enter drains.                                                                                                                                                                                   |
| Methods and materials for containment and cleaning up | : Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10).<br>Take up carefully. Dispose of properly. Clean up affected area.<br>Avoid generation of dusts. |

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

|                                           |                                                                                                                                                   |
|-------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| Further information on storage conditions | : Tightly closed.<br>Dry.<br>Keep in a well-ventilated place.<br>Keep locked up or in an area accessible only to qualified or authorised persons. |
| Storage class                             | : 6.1C, Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects                                               |
| Recommended storage temperature           | : 36 - 46 °F / 2 - 8 °C                                                                                                                           |
| Further information on storage stability  | : Store under argon.                                                                                                                              |

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

### Personal protective equipment

Respiratory protection : required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying

standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type P3

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

#### Hand protection

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.11 mm  
Protective index : Full contact  
Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.11 mm  
Protective index : Splash contact  
Manufacturer : KCL 741 Dermatril® L

Remarks : Handle with impervious gloves.  
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).  
Safety glasses

Skin and body protection : protective clothing

Hygiene measures : Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : solid

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|                                                     |                     |
|-----------------------------------------------------|---------------------|
| Color                                               | : No data available |
| Odor                                                | : No data available |
| Odor Threshold                                      | : No data available |
| pH                                                  | : No data available |
| Melting point                                       | : No data available |
| Boiling point/boiling range                         | : No data available |
| Flash point                                         | : Not applicable    |
| Evaporation rate                                    | : No data available |
| Flammability (solid, gas)                           | : No data available |
| Flammability (liquids)                              | : No data available |
| Burning rate                                        | : No data available |
| Upper explosion limit /<br>Upper flammability limit | : No data available |
| Lower explosion limit /<br>Lower flammability limit | : No data available |
| Vapor pressure                                      | : No data available |
| Relative vapour density                             | : No data available |
| Relative density                                    | : No data available |
| Density                                             | : No data available |
| Water solubility                                    | : No data available |
| Partition coefficient: n-<br>octanol/water          | : No data available |
| Autoignition temperature                            | : No data available |
| Decomposition<br>temperature                        | : No data available |
| Viscosity, dynamic                                  | : No data available |
| Viscosity, kinematic                                | : No data available |
| Flow time                                           | : No data available |

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada



|                          |                                |
|--------------------------|--------------------------------|
| Explosive properties     | : Not classified as explosive. |
| Oxidizing properties     | : none                         |
| Molecular weight         | : 373.20 g/mol                 |
| Particle characteristics |                                |
| Particle size            | : No data available            |

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## SECTION 10. STABILITY AND REACTIVITY

|                                    |                                                                                                                                                                                             |
|------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Reactivity                         | : The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed. |
| Chemical stability                 | : The product is chemically stable under standard ambient conditions (room temperature) .                                                                                                   |
| Possibility of hazardous reactions | : Violent reactions possible with: strong oxidising agents                                                                                                                                  |
| Conditions to avoid                | : no information available                                                                                                                                                                  |
| Incompatible materials             | : No data available                                                                                                                                                                         |
| Hazardous decomposition products   | : In the event of fire: see section 5                                                                                                                                                       |

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## SECTION 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 50 - 300 mg/kg

Remarks: The value is given in analogy to the following substances: 3-Bromo-6-fluoro-2-methyl-1-(1H-1,2,4-triazol-5-ylsulfonyl)-1H-indole

Inhalation: No data available

Dermal: No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

No data available

### **Carcinogenicity**

- IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
- NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
- OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

### **Reproductive toxicity**

Suspected of damaging fertility.  
Suspected of damaging the unborn child.

### **Specific target organ toxicity - single exposure**

No data available

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

No data available

## **11.2 Additional Information**

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## **SECTION 12. ECOLOGICAL INFORMATION**

### **Ecotoxicity**

#### **Components:**

#### **3-Bromo-6-fluoro-2-methyl-1-((1-methyl-1H-1,2,4-triazol-3-yl)sulfonyl)-1H-indole:**

Toxicity to fish : LC50 (Cyprinus carpio (Carp)): 0.232 mg/l  
End point: mortality  
Exposure time: 96 h  
Remarks: The value is given in analogy to the following substances:  
The value is given in analogy to the following substances: 3-Bromo-6-fluoro-2-methyl-1-(1H-1,2,4-triazol-5-ylsulfonyl)-1H-indole

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 4.39 mg/l  
Exposure time: 48 h  
Test Type: static test  
Remarks: The value is given in analogy to the following substances:  
The value is given in analogy to the following substances: 3-Bromo-6-fluoro-2-methyl-1-(1H-1,2,4-triazol-5-ylsulfonyl)-1H-indole

Toxicity to algae/aquatic : EbC50 (Pseudokirchneriella subcapitata): 1.34 mg/l

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plants

Exposure time: 72 h  
Test Type: static test  
Remarks: The value is given in analogy to the following substances:  
The value is given in analogy to the following substances: 3-Bromo-6-fluoro-2-methyl-1-(1H-1,2,4-triazol-5-ylsulfonyl)-1H-indole

ErC50 (*Pseudokirchneriella subcapitata*): 3.28 mg/l  
Exposure time: 72 h  
Test Type: static test  
Remarks: The value is given in analogy to the following substances:  
The value is given in analogy to the following substances: 3-Bromo-6-fluoro-2-methyl-1-(1H-1,2,4-triazol-5-ylsulfonyl)-1H-indole

M-Factor (Acute aquatic toxicity) : 1

Toxicity to fish (Chronic toxicity) : NOEC (*Pimephales promelas* (fathead minnow)): 0.16 mg/l  
Exposure time: 28 d  
Test Type: Growth inhibition  
Remarks: The value is given in analogy to the following substances:  
The value is given in analogy to the following substances: 3-Bromo-6-fluoro-2-methyl-1-(1H-1,2,4-triazol-5-ylsulfonyl)-1H-indole

#### **Persistence and degradability**

No data available

#### **Bioaccumulative potential**

No data available

#### **Mobility in soil**

No data available

#### **Other adverse effects**

##### **Product:**

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances  
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

#### **Endocrine disrupting properties**

No data available

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## SECTION 13. DISPOSAL CONSIDERATIONS

### Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14. TRANSPORT INFORMATION

### International Regulations

#### IATA-DGR

UN/ID No. : UN 2811  
Proper shipping name : Toxic solid, organic, n.o.s.  
(3-Bromo-6-fluoro-2-methyl-1-((1-methyl-1,2,4-triazol-3-yl)sulfonyl)-indole)  
Class : 6.1  
Packing group : III  
Labels : Division 6.1 - Toxic substances  
Packing instruction (cargo aircraft) : 677  
Packing instruction (passenger aircraft) : 670

#### IMDG-Code

UN number : UN 2811  
Proper shipping name : TOXIC SOLID, ORGANIC, N.O.S.  
(3-Bromo-6-fluoro-2-methyl-1-((1-methyl-1,2,4-triazol-3-yl)sulfonyl)-indole)  
Class : 6.1  
Packing group : III  
Labels : 6.1  
EmS Code : F-A, S-A  
Marine pollutant : yes

### Transport in bulk according to IMO instruments

Not applicable for product as supplied.

### National Regulations

#### 49 CFR

UN/ID/NA number : UN 2811  
Proper shipping name : Toxic solids, organic, n.o.s.  
(3-Bromo-6-fluoro-2-methyl-1-((1-methyl-1,2,4-triazol-3-yl)sulfonyl)-indole)  
Class : 6.1  
Packing group : III  
Labels : Division 6.1 - Toxic substances  
ERG Code : 154

Marine pollutant : no  
Poison Inhalation Hazard : No

### Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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## SECTION 15. REGULATORY INFORMATION

### CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

### SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

### SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

**SARA 313** : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489).

### Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

### US State Regulations

#### Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

#### Maine Chemicals of High Concern

Product does not contain any listed chemicals

#### Vermont Chemicals of High Concern

Product does not contain any listed chemicals

### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

### **The components of this product are reported in the following inventories:**

US TSCA : Product contains substance(s) not listed on TSCA inventory.

### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## **SECTION 16. OTHER INFORMATION**

### **Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United

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States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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