

# SAFETY DATA SHEET

according to the OSHA  
Hazard Communication Standard

Version 6.7  
Revision Date 05/18/2026  
Print Date 05/19/2026

## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : I-CBP112

Product Number : SML1134  
Brand : Sigma

### 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**

Short-term (acute) : Category 1

aquatic hazard

Long-term (chronic) aquatic hazard : Category 1

### Other hazards

None known.

### GHS label elements

Hazard pictograms :



Signal word : Warning

Hazard statements : H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**  
P273 Avoid release to the environment.  
**Response:**  
P391 Collect spillage.  
**Disposal:**  
P501 Dispose of contents/ container to an approved waste disposal plant.

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## SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : Not Assigned

### Components

| Chemical name                                                                                                                | CAS No./Unique ID | Concentration (% w/w) | Trade secret |
|------------------------------------------------------------------------------------------------------------------------------|-------------------|-----------------------|--------------|
| 1-[7-(3,4-Dimethoxyphenyl)-9-[[[(3S)--1-methylpiperidin-3-yl]methoxy]-2,3,4,5-tetrahydr-o-1,4-benzoxazepin-4-yl]propan-1-one | -                 | >= 90 - <= 100        | -            |

Actual concentration is withheld as a trade secret

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## SECTION 4. FIRST AID MEASURES

|                                                             |                                                                                                                       |
|-------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------|
| If inhaled                                                  | : After inhalation: fresh air.                                                                                        |
| In case of skin contact                                     | : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.             |
| In case of eye contact                                      | : After eye contact: rinse out with plenty of water. Remove contact lenses.                                           |
| If swallowed                                                | : After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.                  |
| 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<br>Foam<br>Carbon dioxide (CO <sub>2</sub> )<br>Dry powder                                        |
| Unsuitable extinguishing media        | : For this substance/mixture no limitations of extinguishing agents are given.                            |
| Specific hazards during fire fighting | : Combustible.<br><br>Development of hazardous combustion gases or vapours possible in the event of fire. |
| Hazardous combustion products         | : Carbon oxides<br><br>Nitrogen oxides (NO <sub>x</sub> )                                                 |
| 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 : In the event of fire, wear self-contained breathing apparatus.

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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.  
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).  
Take up dry. Dispose of properly. Clean up affected area. 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.  
Dry.

Storage class : 11, Combustible Solids

Recommended storage temperature : 36 - 46 °F / 2 - 8 °C

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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 P1

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

Hygiene measures : Change contaminated clothing. Wash hands after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

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|                                                     |                     |
|-----------------------------------------------------|---------------------|
| Appearance                                          | : solid             |
| 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                                         | : No data available |
| 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          | : log Pow: 3.604    |
| 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 |
| Explosive properties     | : No data available |
| Oxidizing properties     | : none              |
| Molecular weight         | : 468.59 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 | : No data available                                                                                                                                                                         |
| Conditions to avoid                | : no information available                                                                                                                                                                  |
| Incompatible materials             | : Strong oxidizing agents                                                                                                                                                                   |
| 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

Oral: No data available

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

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- 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**

No data available

**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:**

**1-[7-(3,4-Dimethoxyphenyl)-9-[[[(3S)--1-methylpiperidin-3-yl]methoxy]-2,3,4,5-tetrahydr-o-1,4-benzoxazepin-4-yl]propan-1-one:**

Toxicity to fish : Remarks: No data available

M-Factor (Acute aquatic toxicity) : 10

**Persistence and degradability**

No data available

**Bioaccumulative potential**

**Components:**

**1-[7-(3,4-Dimethoxyphenyl)-9-[[[(3S)--1-methylpiperidin-3-yl]methoxy]-2,3,4,5-tetrahydr-o-1,4-benzoxazepin-4-yl]propan-1-one:**

Partition coefficient: n-octanol/water : log Pow: 3.604

**Mobility in soil**

No data available

**Other adverse effects**

No data available

**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 3077  
Proper shipping name : Environmentally hazardous substance, solid, n.o.s.  
(Dimethoxyphenylmethylpiperidinylmethoxytetrahydro benzoxazepinylpropanone)  
Class : 9  
Packing group : III  
Labels : Class 9 - Miscellaneous dangerous substances and articles  
Packing instruction (cargo aircraft) : 956  
Packing instruction (passenger aircraft) : 956

**IMDG-Code**

UN number : UN 3077  
Proper shipping name : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.  
(Dimethoxyphenylmethylpiperidinylmethoxytetrahydro benzoxazepinylpropanone)  
Class : 9  
Packing group : III  
Labels : 9  
EmS Code : F-A, S-F  
Marine pollutant : yes

**Transport in bulk according to IMO instruments**

Not applicable for product as supplied.

**National Regulations****49 CFR**

Not regulated as a dangerous good

Poison Inhalation Hazard : No

### Special precautions for user

Remarks : EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids. Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

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 311/312 Hazards** : No SARA Hazards

**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.

### 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 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

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