

# • SAFETY DATA SHEET

Version 6.9  
Revision Date 03/05/2026  
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## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : Xanthine  
Product Number : X0626  
Brand : Sigma  
CAS-No. : 69-89-6

### 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

Not a hazardous substance or mixture.

**Other hazards**

None known.

**GHS label elements**

Not a hazardous substance or mixture.

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**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Substance / Mixture : Substance

CAS-No. : 69-89-6

**Components**

No hazardous ingredients

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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**

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

Hazardous combustion products : Carbon oxides  
Nitrogen oxides (NO<sub>x</sub>)

Specific extinguishing methods : No data available

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- 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 : Recommended storage temperature see product label.

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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 : Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.11 mm  
Protective index : Splash contact  
Manufacturer : Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Manufacturer : data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

Remarks : Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

- 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

- 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 /  
Upper flammability limit : No data available
- Lower explosion limit /  
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- : No data available

octanol/water

Autoignition temperature : No data available

Decomposition 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 : No data available

Molecular weight : 152.11 g/mol

Particle characteristics  
Particle size : No data available

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## SECTION 10. STABILITY AND REACTIVITY

Reactivity : No data available

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

No data available

#### Skin corrosion/irritation

Remarks: No data available

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**Serious eye damage/eye irritation**

Remarks: No data available

**Respiratory or skin sensitization**

No data available

**Germ cell mutagenicity**

Test Type: Mutagenicity (mammal cell test):

Result: negative

**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**

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**

RTECS: ZD7700000

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

Chronic uptake results in damage of:

Kidney

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Substance which occurs in the human body under physiological conditions.

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**SECTION 12. ECOLOGICAL INFORMATION****Ecotoxicity**

No data available

**Persistence and degradability**

No data available

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

The logo for MilliporeSigma, featuring the word "MILLIPORE" in a bold, red, sans-serif font above the word "SIGMA" in a similar bold, red, sans-serif font.

**Bioaccumulative potential**

No data available

**Mobility in soil**

No data available

**Other adverse effects**

No data available

**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.

**SECTION 14. TRANSPORT INFORMATION****International Regulations****IATA-DGR**

Not regulated as a dangerous good

**IMDG-Code**

Not regulated as a dangerous good

**Transport in bulk according to IMO instruments**

Not applicable for product as supplied.

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

Not regulated as a dangerous good

Poison Inhalation Hazard : No

**Special precautions for user**

Remarks : Not classified as dangerous in the meaning of transport regulations.

**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**

Components	CAS-No.	Component TPQ (lbs)
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**SARA 311/312 Hazards** : Acute Health Hazard

**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 : All substances listed as active on the 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

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