

## SAFETY DATA SHEET

Version 6.6  
Revision Date 08/06/2024  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : *m*-Xylylene diisocyanate

Product Number : 95755  
Brand : Aldrich  
CAS-No. : 3634-83-1

**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**

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

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226  
Acute toxicity, Inhalation (Category 2), H330  
Skin irritation (Category 2), H315  
Serious eye damage (Category 1), H318

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Respiratory sensitization (Category 1), H334  
 Skin sensitization (Sub-category 1A), H317  
 Specific target organ toxicity - single exposure, Inhalation (Category 1), Respiratory Tract, H370  
 Specific target organ toxicity - repeated exposure, Inhalation (Category 1), Respiratory Tract, H372  
 Short-term (acute) aquatic hazard (Category 3), H402  
 Long-term (chronic) aquatic hazard (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H226	Flammable liquid and vapor.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H330	Fatal if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H370	Causes damage to organs (Respiratory Tract) if inhaled.
H372	Causes damage to organs (Respiratory Tract) through prolonged or repeated exposure if inhaled.
H412	Harmful to aquatic life with long lasting effects.

Precautionary Statements

P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P260	Do not breathe mist or vapors.
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.
P272	Contaminated work clothing must not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P284	Wear respiratory protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue

P307 + P311	rinsing. Immediately call a POISON CENTER/ doctor.
P333 + P313	IF exposed: Call a POISON CENTER or doctor/ physician.
P342 + P311	If skin irritation or rash occurs: Get medical advice/ attention.
	If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Lachrymator.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms	: 1,3-Bis(isocyanatomethyl)benzene
Formula	: C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>
Molecular weight	: 188.18 g/mol
CAS-No.	: 3634-83-1
EC-No.	: 222-852-4

Component	Classification	Concentration
<b>1,3-Xylylene diisocyanate</b>		
	Flam. Liq. 3; Acute Tox. 2; Skin Irrit. 2; Eye Dam. 1; Resp. Sens. 1; Skin Sens. 1A; STOT SE 1; STOT RE 1; Aquatic Acute 3; Aquatic Chronic 3; H226, H330, H315, H318, H334, H317, H370, H372, H402, H412	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

No data available

### 4.2 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

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#### **4.3 Indication of any immediate medical attention and special treatment needed**

No data available

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### **SECTION 5: Firefighting measures**

#### **5.1 Extinguishing media**

No data available

#### **5.2 Special hazards arising from the substance or mixture**

Carbon oxides

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

Hydrogen cyanide (hydrocyanic acid)

Combustible.

#### **5.3 Advice for firefighters**

No data available

#### **5.4 Further information**

No data available

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### **SECTION 6: Accidental release measures**

#### **6.1 Personal precautions, protective equipment and emergency procedures**

For personal protection see section 8.

#### **6.2 Environmental precautions**

No data available

#### **6.3 Methods and materials for containment and cleaning up**

No data available

#### **6.4 Reference to other sections**

For disposal see section 13.

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### **SECTION 7: Handling and storage**

#### **7.1 Precautions for safe handling**

For precautions see section 2.2.

#### **7.2 Conditions for safe storage, including any incompatibilities**

**Storage stability** Recommended storage temperature

2 - 8 °C

Light sensitive. Store under inert gas. Moisture sensitive. Exposure to moisture.

**Storage class**

Storage class (TRGS 510): 3: Flammable liquids

#### **7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

No data available

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |   |   |
|---|---|
| a) Appearance                                   | Form: liquid<br>Color: light yellow                           |
| b) Odor   | No data available   |
| c) Odor Threshold                               | No data available   |
| d) pH   | No data available   |
| e) Melting point/freezing point                 | Melting point/ range: -7 °C (19 °F) - OECD Test Guideline 102 |
| f) Initial boiling point and boiling range      | 88 - 90 °C 190 - 194 °F at 0.03 hPa                           |
| g) Flash point                                  | 42 °C (108 °F) - closed cup                                   |
| h) Evaporation rate                             | No data available   |
| i) Flammability (solid, gas)                    | No data available   |
| j) Upper/lower flammability or explosive limits | No data available   |
| k) Vapor pressure                               | < 0.1 hPa at 20 °C (68 °F) - OECD Test Guideline 104          |
| l) Vapor density                                | No data available   |
| m) Density                                      | 1.202 g/mL at 20 °C (68 °F)                                   |
| Relative density                                | 1.220 °C - OECD Test Guideline 109                            |
| n) Water solubility                             | No data available   |
| o) Partition coefficient: n-octanol/water       | No data available   |
| p) Autoignition temperature                     | No data available   |
| q) Decomposition temperature                    | No data available   |
| r) Viscosity                                    | No data available   |
| s) Explosive properties                         | No data available   |

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t) Oxidizing properties none

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

No data available

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Amines, Alcohols, Strong oxidizing agents

### 10.6 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 - male and female - 3,200 mg/kg  
(OECD Test Guideline 401)

Acute toxicity estimate Inhalation - Expert judgment - 4 h - 0.51 mg/l - vapor

LD50 Dermal - Rat - male and female - > 2,000 mg/kg  
(OECD Test Guideline 402)

#### Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 4 h  
(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage.  
(OECD Test Guideline 405)

#### Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: positive

(OECD Test Guideline 406)

May cause allergic respiratory and skin reactions

**Germ cell mutagenicity**

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: positive

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Micronucleus test

Species: Rat

Cell type: Bone marrow

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

**Carcinogenicity**

IARC: No ingredient 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 ingredient 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**

Inhalation - Causes damage to organs. - Respiratory Tract

**Specific target organ toxicity - repeated exposure**

Inhalation - Causes damage to organs through prolonged or repeated exposure.

- Respiratory Tract

**Aspiration hazard**

No data available

**11.2 Additional Information**

Repeated dose toxicity - Rat - male and female - Oral - NOAEL (No observed adverse effect level) - 50 mg/kg

RTECS: NR0147000

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

### 12.1 Toxicity

Toxicity to fish	semi-static test LC50 - <i>Oryzias latipes</i> (Japanese medaka) - 87.6 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> - 31.5 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	

### 12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 0 % - Not readily biodegradable. (OECD Test Guideline 301C)
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### 12.3 Bioaccumulative potential

No data available

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

### 12.6 Endocrine disrupting properties

No data available

### 12.7 Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

No data available

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## SECTION 14: Transport information

#### DOT (US)

UN number: 2920    Class: 8 (3)    Packing group: II  
Proper shipping name: Corrosive liquids, flammable, n.o.s. (1,3-Xylylene diisocyanate)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### IMDG

UN number: 2920    Class: 8 (3)    Packing group: II    EMS-No: F-E, S-C

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Proper shipping name: CORROSIVE LIQUID, FLAMMABLE, N.O.S. (1,3-Xylylene diisocyanate)

**IATA**

UN number: 2920 Class: 8 (3)

Packing group: II

Proper shipping name: Corrosive liquid, flammable, n.o.s. (1,3-Xylylene diisocyanate)

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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**

: Fire Hazard

**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 ingredients of this product are reported in the following inventories:**

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**

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

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