

## SAFETY DATA SHEET

Version 6.10  
Revision Date 10/27/2023  
Print Date 04/28/2024

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Toluene-2,4-diisocyanate

Product Number : 216836  
Brand : Aldrich  
Index-No. : 615-006-00-4  
CAS-No. : 584-84-9

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

Identified uses : Laboratory chemicals, Synthesis of substances

**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)**

Acute toxicity, Inhalation (Category 1), H330  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Respiratory sensitization (Category 1), H334  
Skin sensitization (Category 1), H317  
Carcinogenicity (Category 2), H351  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335  
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 statement(s)

H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H319	Causes serious eye irritation.
H330	Fatal if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H335	May cause respiratory irritation.
H351	Suspected of causing cancer.
H412	Harmful to aquatic life with long lasting effects.

Precautionary statement(s)

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P260	Do not breathe mist or vapors.
P264	Wash skin thoroughly after handling.
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/ protective clothing/ eye protection/ face protection.
P284	Wear respiratory protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P342 + P311	If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.
P362	Take off contaminated clothing and wash 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 Hazards not otherwise classified (HNOC) or not covered by GHS

Lachrymator.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : TDI  
4-Methyl-1,3-phenylene diisocyanate  
2,4-Diisocyanatotoluene  
4-Methyl-m-phenylene diisocyanate  
Toluene 2,4-diisocyanate

Formula :  $C_9H_6N_2O_2$   
Molecular weight : 174.16 g/mol  
CAS-No. : 584-84-9  
EC-No. : 209-544-5  
Index-No. : 615-006-00-4

Component	Classification	Concentration
<b>4-methyl-m-phenylene diisocyanate</b>		
	Acute Tox. 1; Skin Irrit. 2; Eye Irrit. 2A; Resp. Sens. 1; Skin Sens. 1; Carc. 2; STOT SE 3; Aquatic Acute 3; Aquatic Chronic 3; H330, H315, H319, H334, H317, H351, H335, H402, H412 Concentration limits: >= 0.1 %: Resp. Sens. 1, H334;	<= 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

#### General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

#### 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**

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

**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

**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****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.

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

Carbon oxides

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

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

**5.3 Advice for firefighters**

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

**5.4 Further information**

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

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

**6.2 Environmental precautions**

Do not let product enter drains.

**6.3 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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

## 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

#### Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

#### Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

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

#### Storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

#### Storage stability

Recommended storage temperature

2 - 8 °C

Store under inert gas. Product is sensitive to light and moisture.

#### Storage class

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

### 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

Component	CAS-No.	Value	Control parameters	Basis
	Remarks	Potential Occupational Carcinogen See Appendix A		
4-methyl-m-phenylene diisocyanate	584-84-9	TWA	0.0050 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Eye irritation Asthma Respiratory sensitization Adopted values or notations enclosed are those for which changes are proposed in the NIC See Notice of Intended Changes (NIC)		

		Not classifiable as a human carcinogen Sensitizer		
		STEL	0.02 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Eye irritation Asthma Respiratory sensitization Adopted values or notations enclosed are those for which changes are proposed in the NIC See Notice of Intended Changes (NIC) Not classifiable as a human carcinogen Sensitizer		
		C	0.02 ppm 0.14 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate. Ceiling limit is to be determined from breathing-zone air samples.		
		TWA	0.0050 ppm 0.04 mg/m3	USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)
		STEL	0.02 ppm 0.15 mg/m3	USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)

#### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
4-methyl-m-phenylene diisocyanate	584-84-9	toluene diamine	5µg/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift			

## 8.2 Exposure controls

### Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

### Personal protective equipment

#### Eye/face protection

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

#### Skin protection

required

#### Body Protection

protective clothing

#### Respiratory protection

Recommended Filter type: Filter type ABEK

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.  
required when vapours/aerosols 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.

### **Control of environmental exposure**

Do not let product enter drains.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

a) Appearance	Form: clear, liquid Color: colorless
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 20 - 22 °C (68 - 72 °F) - lit.
f) Initial boiling point and boiling range	115 - 120 °C 239 - 248 °F at 13 hPa - lit.
g) Flash point	132 °C (270 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 9.5 %(V) Lower explosion limit: 0.9 %(V)
k) Vapor pressure	0.04 hPa at 25 °C (77 °F)
l) Vapor density	6.01 - (Air = 1.0)
m) Density	1.225 g/cm <sup>3</sup> at 25 °C (77 °F)
Relative density	1.2125 °C - Regulation (EC) No. 440/2008, Annex, A.3
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	log Pow: 3.43 at 22 °C (72 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available

- r) Viscosity No data available
- s) Explosive properties No data available
- t) Oxidizing properties none

## 9.2 Other safety information

Surface tension	25 mN/m at 25 °C (77 °F)
Relative vapor density	6.01 - (Air = 1.0)

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Heat.  
Strong heating.

### 10.5 Incompatible materials

Alcohols, Strong bases, Amines, acids, 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 - 5,110 mg/kg  
(OECD Test Guideline 401)

Remarks: (in analogy to similar compounds)

The value is given in analogy to the following substances: m-tolylidene diisocyanate  
LC50 Inhalation - Rat - male and female - 4 h - 0.12 mg/l - vapor

(OECD Test Guideline 403)

Remarks: (in analogy to similar products)

Inhalation: Irritating to respiratory system.

LD50 Dermal - Rabbit - male and female - > 9,400 mg/kg  
(OECD Test Guideline 402)

Remarks: (in analogy to similar products)

The value is given in analogy to the following substances: m-tolylidene diisocyanate



No data available

### **Skin corrosion/irritation**

Skin - Rabbit

Result: Irritating to skin. - 24 h

Remarks: (RTECS)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Irritating to eyes.

(Draize Test)

Remarks: (ECHA)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

### **Respiratory or skin sensitization**

Open epicutaneous test - Guinea pig

Result: positive

Remarks: (ECHA)

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

May cause allergy or asthma symptoms or breathing difficulties if inhaled. Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

### **Germ cell mutagenicity**

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: positive

Test Type: In vivo micronucleus test

Species: Rat

Application Route: Inhalation

Method: Mutagenicity (micronucleus test)

Result: negative

Test Type: unscheduled DNA synthesis assay

Species: Rat

Application Route: Inhalation

Result: negative

Remarks: (ECHA)

Test Type: Micronucleus test

Species: Mouse

Application Route: Inhalation

Method: OECD Test Guideline 474

Result: negative

### **Carcinogenicity**

Suspected of causing cancer.

- IARC: 2B - Group 2B: Possibly carcinogenic to humans (4-methyl-m-phenylene diisocyanate)
- NTP: RAHC - Reasonably anticipated to be a human carcinogen (4-methyl-m-phenylene diisocyanate)
- 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 - May cause respiratory irritation. - Respiratory Tract

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

RTECS: CZ6300000

Cough, Shortness of breath, Headache, Nausea, Vomiting

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

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

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**SECTION 12: Ecological information**

**12.1 Toxicity**

Toxicity to fish	static test LC50 - Oncorhynchus mykiss (rainbow trout) - 133 mg/l - 96 h (OECD Test Guideline 203) Remarks: (in analogy to similar products)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 12.5 mg/l - 48 h (OECD Test Guideline 202) Remarks: (in analogy to similar products)
Toxicity to algae	EC50 - Skeletonema costatum (marine diatom) - 3,230 mg/l - 96 h (OECD Test Guideline 201) Remarks: (in analogy to similar products)
Toxicity to bacteria	EC50 - activated sludge - > 100 mg/l - 3 h (OECD Test Guideline 209)

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Remarks: (in analogy to similar products)

Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) static test EC50 - Daphnia magna (Water flea) - 2 mg/l - 21 d (OECD Test Guideline 211)  
Remarks: (in analogy to similar products)

#### 12.2 Persistence and degradability

Biodegradability aerobic Biochemical oxygen demand - Exposure time 28 d  
Result: 0 % - Not biodegradable  
(OECD Test Guideline 302C)  
Remarks: (in analogy to similar compounds)

#### 12.3 Bioaccumulative potential

Bioaccumulation Cyprinus carpio (Carp) - 60 d  
at 24.8 °C - 0.8 mg/l(4-methyl-m-phenylene diisocyanate)  
  
Bioconcentration factor (BCF): 180  
(OECD Test Guideline 305)

#### 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

##### Product

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

#### DOT (US)

UN number: 2078 Class: 6.1

Packing group: II

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Proper shipping name: Toluene diisocyanate  
Reportable Quantity (RQ): 100 lbs  
Poison Inhalation Hazard: No

**IMDG**

UN number: 2078    Class: 6.1    Packing group: II    EMS-No: F-A, S-A  
Proper shipping name: TOLUENE DIISOCYANATE

**IATA**

UN number: 2078    Class: 6.1    Packing group: II  
Proper shipping name: Toluene diisocyanate

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**SECTION 15: Regulatory information**

**SARA 302 Components**

4-methyl-m-phenylene diisocyanate	CAS-No. 584-84-9	Revision Date 1993-04-24
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**SARA 313 Components**

The following components are subject to reporting levels established by SARA Title III, Section 313:

4-methyl-m-phenylene diisocyanate	CAS-No. 584-84-9	Revision Date 1993-04-24
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**SARA 311/312 Hazards**

Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

4-methyl-m-phenylene diisocyanate	CAS-No. 584-84-9	Revision Date 1993-04-24
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**Pennsylvania Right To Know Components**

4-methyl-m-phenylene diisocyanate	CAS-No. 584-84-9	Revision Date 1993-04-24
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## SECTION 16: Other information

### Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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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