

## GPS Safety Summary

**TDI, Toluene diisocyanate,  
covers the following commercial products:**

**a) mixed TDI isomers (CAS 26471-62-5) composed  
of 65-80 % 2,4-TDI isomer (CAS 584-84-9) and  
20 – 35 % 2,6-TDI isomer (CAS 91-08-7)**

**b) pure 2,4-TDI isomer (CAS 584-84-9)**

“TDI” (Toluene diisocyanate), is commercially available in three different grades, dependent on the ratio of its two isomers, 2,4-TDI and 2,6-TDI.

The pure 2,4-Isomer is commercially available as “TDI 100”, which is a colorless to pale yellow solid at room temperature with a melting point of 21.8°C.

The pure 2,6-Isomer is a colorless to pale yellow liquid at room temperature with a melting point of 8°C .

The most used isomer mixture contains 80% of the 2,4-isomer and 20% 2,6-isomer, is a clear, colorless to pale yellow liquid with a sharp, pungent odor, and solidifies at 9.5°C. The 2<sup>nd</sup> mixture consists of 65% 2,4-TDI and 35% 2,6-TDI and has a melting point of 4°C.

TDI is one of the commonly used raw materials for Polyurethane manufacturing.. There are several world scale plants around the globe, where these raw materials are manufactured. They all start from toluene over DNT to the corresponding Toluidine base, TDA, which is further converted into the final TDI (pure substance or mixed isomers).

Based on its intrinsic toxicity TDI is exclusively used in industrial and professional applications. Any uses by consumers are strictly advised against.

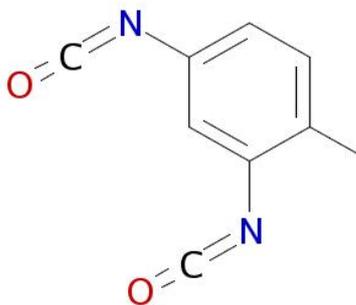
## Chemical Identity

**Name:** Toluene diisocyanate, mixed isomer

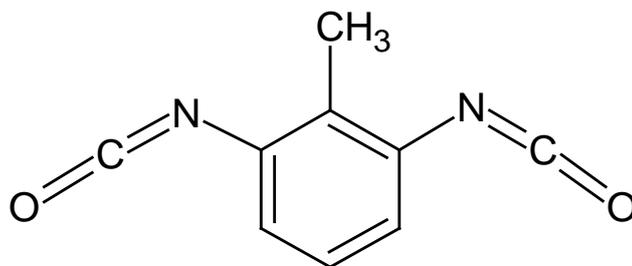
**Brand names:** TDI

|                                   |   |
|-----------------------------------|---|
| <b>EC number:</b>                 | 247-722-4 (isomer mixture); pure 2,4-TDI: EC 209-544-5; pure 2,6-TDI: EC 202-039-0;   |
| <b>EC name:</b>                   | m-tolyldiene diisocyanate   |
| <b>CAS number (EC inventory):</b> | 26471-62-5 (isomer mixture); pure 2,4-TDI: 584-84-9; pure 2,6-TDI: 91-08-7;   |
| <b>CAS name:</b>                  | Benzene, 1,3-diisocyanato methyl- (for isomer mixture); pure 2,4-TDI: Benzene, 2,4-diisocyanato-1-methyl-; pure 2,6-TDI: Benzene, 1,3-diisocyanato-2-methyl-; |
| <b>IUPAC name:</b>                | 2,4-diisocyanato-1-methylbenzene, 2,6-diisocyanato-1-methylbenzene;   |
| <b>Annex I index number:</b>      | 615-006-00-4  |
| <b>Molecular formula:</b>         | C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>   |
| <b>Molecular weight range:</b>    | 174.1561  |

**Structural formula:**



**2,4-TDI Isomer**



**2,6-TDI Isomer**

## Uses and Applications<sup>1</sup>:

Based on the intrinsic toxicity of TDI the exclusive use under controlled conditions is supported.

TDI is used as an intermediate for the synthesis of other chemical substances, utilizing its unique behavior of two reaction groups with different reactivity in the same molecule.

The majority of the global TDI volumes however are exclusively used in Polyurethanes in order to manufacture finished parts, such as foams, cast elastomers, adhesives, sealants, fibers and also some composites for other materials. The by far biggest application of toluene diisocyanates are flexible Polyurethanes, both, slabstock and molded foams. These foams find applications as automotive cushions, carpet underlay, furniture, seating and bedding.

## Physical/Chemical Properties

### Phys/Chem Safety Assessment:

Toluene diisocyanate, is a clear, colorless to pale yellow liquid with a sharp, pungent odor. Dependent on its isomer ratio, its melting point is 9.5° C (2,4-isomer/2,6-isomer = 80/20) or 4°C for the corresponding 65/35 ratio.

### Overview of physico-chemical properties

| Property       | Value  |
|----------------|--|
| Form           | substance, mixture of two isomers  |
| Physical state | liquid at 20°C and 1013 hPa  |
| Melting point  | The melting point of 80:20 TDI is 9.5°C and that of 65:35 TDI is 4°C.<br>pure 2,4-TDI: 21.8°C; pure 2,6-TDI: 8°C |
| Boiling point  | A boiling range of 252°C to 254°C was determined for 80:20 TDI, and a range of 253°C to 255°C for 65:35 TDI.     |
| Color          | colourless to pale yellow  |
| Odor           | sharp pungent  |

<sup>1</sup> Reference is made to:

1. Kirk-Othmer, Encyclopedia of Chemical Technology, and there "Organic Isocyanates", John Wiley & Sons, 2000
2. Both, the pure 2,4-TDI isomer and its mixtures with 2,6-TDI isomer have been registered under REACH. The information provided with the corresponding technical dossiers is referenced to in this safety summary.

| <b>Property</b>  | <b>Value</b>  |
|--|---|
| <b>Relative density</b>                                  | At 20°C the relative density of 80:20 TDI and of 65:35 TDI was determined as 1.22   |
| <b>Vapor pressure</b>                                    | The vapor pressure of 80:20 TDI at 20°C was calculated as 0.015 hPa, and that of 65:35 TDI as 0.014 hPa.  |
| <b>Mol weight</b>  | 174.1561  |
| <b>Flammability</b>                                      | Non-flammable. Based on the structural properties of the substance and the experience in handling, no pyrophoricity is expected. The substance does not liberate flammable gases on contact with water  |
| <b>Explosive properties</b>                              | TDI was shown to have no explosive properties.  |
| <b>Self-ignition temperature</b>                         | No auto ignition was observed up to 595°C at 1013hPa.   |
| <b>Water solubility</b>                                  | TDI is hydrolytically unstable. It can have only a transient existence in aqueous media. A water solubility value of 124 mg/l has been estimated (West et al, 2008) using a broadly accepted program, though a water solubility value for TDI is only a notional concept. |
| <b>Flash point</b>                                       | The 80:20 mixture (2,4-TDI: 2,6-TDI) shows a flash point of 132°C, the 65:35 mixture has a flash point of 128°C.  |
| <b>Partition coefficient n-octanol/water (log value)</b> | A log Pow value of 3.43 at 22°C was determined. This is only a theoretical value because TDI is hydrolytically unstable.  |

## Health Effects

Toluene diisocyanate (TDI) is acutely very toxic by inhalation exposure to vapors. Severe irritation of the respiratory tract, of the skin and of the eyes is the predominant acute health effect. Likewise the strong irritating potential at the portal of entry should be taken into account for acute oral exposures.

TDI poses a strong sensitizing potential to both skin and respiratory tract.

Sensitization of the respiratory tract may result in significant decreases in lung function in workers, an asthma-like reaction characterized by wheezing, dyspnea, and bronchial constriction. Animal studies and/or human evidence suggest that respiratory sensitization might also occur after skin contact.

Toxicity following repeated exposure occurs locally at the site of contact. Repeated exposure to TDI vapors is resulting in irritation of the respiratory tract, no signs of systemic toxicity were observed in animal studies.

Tests assessing the mutagenic potential of TDI *in vitro* and *in vivo* provide no consistent evidence for a genotoxic activity. Chronic studies conducted on rodents indicated that oral exposure may result in tumor formation. However the mechanism of tumor formation has shown to be not relevant for the inhalation route of exposure. Concordantly no indications for a carcinogenic potential were described in humans exposed to TDI vapors. Studies conducted in rats indicated that TDI vapors are not toxic to fertility or development.

**We therefore exclusively support the industrial/professional use only.**

## Human Health Safety Assessment

- **Industrial Workers:** Exposure is very unlikely as TDI is manufactured and handled in industrial facilities and settings in closed systems under strictly controlled conditions only.  
For manufacturing rigorous containment by technical means are applied. In case of unintended exposure due to accidents, appropriate Risk Management Measures are in place.
- **Professional workers:** Exposure is unlikely, as TDI must be handled under strictly controlled conditions with corresponding PPE. In case of unintended exposure due to accidents, appropriate Risk Management Measures are in place.
- **Consumer: Not supported.**

| <b>Effect Assessment</b>   | <b>Result</b>   |
|--|---|
| <b>Acute Toxicity<br/>oral / inhalation / dermal</b>                   | Fatal if inhaled.<br>Acute Toxicity Cat. 1  |
| <b>Irritation / corrosion<br/>skin / eye / respiratory tract</b>       | Highly irritating for skin, eyes and the respiratory tract.<br>Skin Irritation Cat. 2<br>Eye irritation Cat. 2A<br>STOT SE-Cat 3 for respiratory tract irritation |
| <b>Sensitization</b>   | Strong sensitizer to skin and respiratory tract.<br>Skin Sensitization Cat. 1<br>Respiratory Sensitization Cat. 1   |
| <b>Toxicity after repeated exposure<br/>oral / inhalation / dermal</b> | Local irritation at site of contact. Not classified for systemic toxicity following repeated exposure.  |
| <b>Genotoxicity / Mutagenicity</b>                                     | Not classified as mutagenic.  |
| <b>Carcinogenicity</b>   | Suspected of causing cancer on the oral route of exposure.<br>Carcinogenicity Cat.2   |
| <b>Toxicity for reproduction</b>                                       | Not classified as toxic to reproduction   |

## Environmental Effects

**TDI is unstable in aqueous media where it reacts to form predominantly insoluble and inert polyureas.**

**TDI and its hydrolysis products are not readily biodegradable. No bioaccumulation is expected for TDI and the decomposition products.**

**TDI has low to moderate toxicity for aquatic organisms.**

## Environmental Safety Assessment

An in-depth environmental exposure assessment confirmed that TDI<sup>2</sup> can be handled safe during all steps of manufacture and industrial/professional uses.

Industrial facilities and settings are fitted with special equipment, ensuring encapsulation of the substance in closed systems under strictly controlled conditions. Thus, rigorous containment by technical means is applied in manufacturing of TDI .

Due to the fact that manufacturing and uses of the substance are restricted to specific applications with corresponding PPE and strict RMM in place, and usually highly skilled and trained industrial/professional workers are involved, exposures are unlikely.

<sup>2</sup> Reference is made to the registration of the substance under REACH and the provided information with the corresponding IUCLID Dossier.

At manufacturing sites for TDI, waste water is subjected to industrial waste water treatment plant with adapted sludge.

| Effect Assessment | Result   |
|-------------------|--|
| Aquatic Toxicity  | Harmful to aquatic life with long lasting effects. |

| Fate and behavior         | Results   |
|---------------------------|---|
| Biodegradation            | not readily biodegradable (according to OECD criteria).   |
| Bioaccumulation potential | TDI is classified as <b>not</b> potentially bioaccumulating based on the experimental log Kow of 3.43 and is therefore identified as <u><i>not potentially</i></u> B. |
| PBT / vPvB conclusion     | TDI is <b>not</b> classified as PBT and vPvB.   |

## Exposure

### Human health

The exposure potential to TDI is low, since manufacturing and uses are restricted to specially dedicated facilities. All known and identified uses are limited to industrial/professional stages and thus no other than industrial and professional workers with special training and supervision handle the substance.

Since all equipment for manufacturing and transport are completely closed and strictly controlled, the substance is contained under rigorous conditions at least for manufacturing and transport.

It is mandatory that any person who might potentially come into contact with the substance has to wear corresponding PPE (Personal Protective Equipment). In case of any accident, appropriate risk management measures are in place.

### Environment

During manufacturing and transport, the substance is handled under rigorous containment by technical means under strictly controlled conditions. Its uses are limited to special industrial and some professional applications with highly skilled and trained industrial/professional workers only, thus it can be concluded that the risk for exposure of TDI to the environment is low. There are no releases to the environment at industrial facilities, since waste water is treated in industrial waste

water treatment plants with adapted sludge. Any waste is subject to industrial incineration plants.

All identified uses in the industrial and professional segments for TDI have been proved to be safe by an in-depth environmental exposure assessment conducted for TDI during REACH registration<sup>3</sup>.

As TDI rapidly hydrolyses in contact with water (DT50 ranges from 0.5 to 30 min at ambient temperature) the production of TDI is a dry process. Therefore no emissions into water occur at production facilities.

Due to the rapid decomposition in aqueous media an exposure of sediment to TDI is negligible, a risk characterization for this compartment is therefore considered not to be relevant.

## **Risk Management Recommendations**

**We only support the industrial/professional use of TDI under strictly controlled conditions with appropriate PPE respectively.**

**When using the substance, make sure that there is adequate ventilation of stores and work areas. Refill and handle only in closed system.**

### **Precautions for safe handling of TDI**

Provide suitable exhaust ventilation at the processing machines. Ensure thorough ventilation of work areas and stores. Avoid aerosol formation. When handling heated product, vapors of the product should be ventilated and respiratory protection used. Wear respiratory protection, when spraying. Danger of bursting when sealed gastight. Protect against moisture. Products freshly manufactured from isocyanates can contain incompletely reacted isocyanates and other dangerous substances.

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<sup>3</sup> Reference is made to the corresponding IUCLID Dossier and information provided with for the registration under REACH.

## **Personal Protective Equipment**

Reference is made to the use of suitable eye and skin protection.

Suitable personal breathing, eye and skin protection are:

### 1. Respiratory protection:

Personal protective equipment in case of vapour/aerosol release. Gase filter for gases/vapours of organic compounds (boiling point > 65°C, e.g. EN 14387 Type A). Particle filter with high efficiency for solid and liquid particles (e.g. EN 143 or 149, Type P3 or FFP3).

Suitable respiratory protection for higher concentrations or long-term effect: Self-contained breathing apparatus.

### 2. Hand protection:

Chemical resistant protective gloves (EN 374).

Suitable materials also with prolonged, direct contact (recommended: protective index 6, corresponding > 480 minutes of permeation time according to EN 374):

nitrile rubber (NBR) - 0.4 mm coating thickness

butyl rubber (butyl) - 0.7 mm coating thickness

chloroprene rubber (CR) - 0.5 mm coating thickness.

Unsuitable materials:

polyvinylchloride (PVC) - 0.7 mm coating thickness

Polyethylene-Laminate (PE laminate) – ca. 0.1 mm coating thickness.

### 3. Eye protection:

Safety glasses with side-shields (frame goggles) (e.g. EN 166)

### 4. Body protection:

Safety shoes (e.g. according to EN 20346)

## **General safety and hygiene measures:**

Do not breathe vapour/spray. With products freshly manufactured from isocyanates body protection and chemical resistant protective gloves is recommended. Wearing of closed work clothing is required additionally to the stated personal protection equipment. Keep away from food, drink and animal feeding stuffs. No eating, drinking, smoking or tobacco use at the place of work. Take off immediately all contaminated clothing. Hands and /or face should be washed before breaks and at the end of shift. At the end of the shift the skin should be cleaned and skin-care agents applied.

## Environment

As TDI rapidly hydrolyses when in contact with water (DT50 ranges from 0.5 to 30 min at ambient temperature), the production of TDI is a dry process. Therefore the emission factor to waste water is set to 0.

## State Agency Review

TDI has been registered under REACH.

## Regulatory Information/ Classification and Labelling

According to GHS, substances are classified according to their physical, health and environmental hazards. The hazards are communicated via specific labels and the eSDS. GHS attempts to standardize hazard communication so that the intended audience (workers, consumers, transport workers, and emergency responders) can better understand the hazards of the chemical in use.

### Classification and labelling of TDI mixed isomers according to CLP / GHS:

#### Classification:

|                                |  |
|--------------------------------|--|
| Acute toxicity - inhalation:   | Acute Tox. 1 (Hazard statement: H330: Fatal if inhaled.)   |
| Skin corrosion/irritation:     | Skin Irrit. 2 (Hazard statement: H315: Causes skin irritation.)  |
| Serious damage/eye irritation: | Eye Irrit. 2A (Hazard statement: H319: Causes serious eye irritation.)   |
| Respiration sensitization:     | Resp. Sens. 1 (Hazard statement: H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled.) |
| Skin sensitization:            | Skin Sens. 1 (Hazard statement: H317: May cause an allergic skin reaction.)  |

|  |  |
|--|--|
| Carcinogenicity:                         | Carc. 2 (Hazard statement: H351: Suspected of causing cancer; Route of exposure: oral.)        |
| Specific target organ toxicity - single: | STOT Single Exp. 3 (Hazard statement: H335: May cause respiratory irritation.)                 |
| Hazards to the aquatic environment:      | Aquatic chronic 3 (Hazard statement: H412: Harmful to aquatic life with long lasting effects.) |

Specific concentration limits:

| Concentration (%) | Classification |
|-------------------|----------------|
| >= 0.1            | Resp. Sens. 1  |

**Labelling:**

Signal word: Danger

Hazard pictogram:

GHS06: skull and crossbones



GHS08: health hazard



Hazard statements:

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

Precautionary statements:

P273: Avoid release to the environment.

P280: Wear protective gloves/protective clothing/eye protection/face protection.

P284: Wear respiratory protection.

P308+P313: IF exposed or concerned: Get medical advice/attention.

P403+P233: Store in a well-ventilated place. Keep container tightly closed.

P501: Dispose of contents/container to hazardous or special waste collection point.

## Contact information.

### **ISOPA, European Diisocyanate and Polyol Producers Association**

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ISOPA is the European trade association for producers of diisocyanates and polyols - the main building blocks of polyurethanes.

- ISOPA promotes the highest standards of best practice in the distribution and use of diisocyanates and polyols
- ISOPA ensures that all stakeholders can easily access accurate and up-to-date information on diisocyanates and polyols
- ISOPA shows how polyurethanes help fulfil society's present and future needs

<http://www.icca-chem.org/en/Home/ICCA-initiatives/global-product-strategy/>

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**Revision: --**

## Glossary:

|                  |   |
|------------------|---|
| Acute toxicity   | harmful effects after a single exposure                                   |
| Biodegradable    | breakdown of materials by a physiological environment                     |
| Bioaccumulation  | accumulation of substances in the environment                             |
| Carcinogenicity  | effects causing cancer  |
| Chronic toxicity | harmful effects after repeated exposures                                  |
| GHS              | Global Harmonized System  |
| Hazard           | situation bearing a threat to health and environment                      |
| Mutagenicity     | effects that change genes   |
| Reprotoxicity    | combining teratogenicity, embryotoxicity and harmful effects on fertility |
| Sensitising      | allergenic  |

## Disclaimer:

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