

## **TDI Synonyms, Acronyms, and CAS Registry Numbers**

An individual TDI molecule (monomer) can exist in more than one isomeric form. Sometimes TDI is produced to consist of the relatively pure 2,4-TDI isomer. Sometimes TDI is produced as a mixture of isomers as is known as “generic TDI.” Most commonly, generic TDI consists of an 80:20 mixture of the 2,4- and 2,6-TDI isomers, but other mixes are possible. Sometimes TDI is processed so that some of the TDI molecules link together to form homopolymers (dimers, trimers and oligomers).

At least two formal systems of nomenclature are used to describe TDI in its various forms; in addition, many non-systematic names are used. The following summarizes information on these various names. Although a wide range of literature has been reviewed to compile the following, these lists are not necessarily exhaustive. Key sources of information consulted were:

- Chemical Abstracts Service (CAS<sup>TM</sup>) Registry {Online Search}, Columbus, 2000
- Advanced Chemistry Development Inc., ACD/I-Lab web service {IUPAC names}, 2000
- Chemical Manufacturers Association and Society of the Plastics Industry, Inc. Instruction Manual: Nomenclature for Diisocyanate TDI, MDI and Derivatives, 1993
- MDI and TDI Nomenclature, Gilbert International Limited 2001, GIL Report Number 2001/B, B. Tury, D.S. Gilbert, D.C. Allport, January 2001

The third source (Instruction Manual: Nomenclature for Diisocyanate TDI, MDI and Derivatives) provides rules for naming TDI and TDI derivatives for purposes of the Toxic Substances Control Act Chemical Inventory. For information on obtaining that manual, click [here](#) .

### CAS Registry Numbers & Preferred Names

### International Union of Pure and Applied Chemistry (IUPAC) System

### TDI Acronyms

### TDI Synonyms

## A. CAS Registry Numbers & Index/Preferred Names

The Chemical Abstracts Service (CAS) maintains a registry of chemical substances that assigns each chemical a registry number (CASRN) and a unique systematic name. CAS also works with the U.S. Environmental Protection Agency to develop names and CASRNs for substances added to the Toxic Substances Control Act Chemical Inventory. Table A provides CASRNs and CA index or preferred names for various TDI species.

**Table A: CAS Registry Numbers and Index/Preferred Names for TDI Species**

CAS Number	CA Index/Preferred Name	Short Name
584-84-9	benzene, 2,4-diisocyanato-1-methyl-	2,4-TDI
91-08-7	benzene, 1,3-diisocyanato-2-methyl-	2,6-TDI
26471-62-5*	benzene, 1,3-diisocyanatomethyl-*	generic TDI*
3320-33-0	1,3-diazetidone-2,4-dione, 1,3-bis(3-isocyanato-4-methylphenyl)-	2,4-TDI dimer
1321-38-6**	benzene, diisocyanatomethyl**	totally unspecified TDI**
9017-01-0	benzene, 1,3-diisocyanatomethyl-, homopolymer	generic TDI homopolymer
9019-85-6	benzene, 1,3-diisocyanatomethyl-, trimer	generic TDI trimer
26006-20-3	benzene, 2,4-diisocyanato-1-methyl-, homopolymer	2,4-TDI homopolymer
31370-61-3**	benzene, 1,3-diisocyanato-2-methyl-, polymer with 2,4-diisocyanato-1-methylbenzene**	2,4-TDI/2,6-TDI copolymer**

For purposes of the Toxic Substances Control Act, this CASRN and name should be used for all mixtures of 2,4-TDI and 2,6-TDI. See [Instruction Manual: Nomenclature for Diisocyanate TDI, MDI and Derivatives](#)

\*\* For purposes of the Toxic Substances Control Act, this CASRN and name should not be used.

See [Instruction Manual: Nomenclature for Diisocyanate TDI, MDI and Derivatives](#)

## B. International Union of Pure and Applied Chemistry (IUPAC) System

The IUPAC, an international association of chemists, has devised a formal system of chemical nomenclature. Unlike the CAS system, the IUPAC system does not assign unique numbers to chemicals. Also, the IUPAC system does not extend to mixtures of chemicals, as these cannot be defined by a specific structure. Table D lists IUPAC names for TDI species; these names are used primarily in academic literature.

**Table B: TDI IUPAC Nomenclature**

Species	IUPAC Name
2,4-TDI	2,4-diisocyanato-1-methylbenzene
2,6-TDI	1,3-diisocyanato-2-methylbenzene
Generic TDI	No name, because it is a mixture

### C. TDI Acronyms

As can be seen from the above, the formal names for TDI can be unwieldy. Therefore, acronyms are usually used. The following table lists commonly-used acronyms or abbreviations for various forms of TDI. The acronym “TDI” comes from “toluene diisocyanate,” a name commonly used in industry.

**Table C: TDI Acronyms**

Type	Abbreviation	Description	CASRN
Generic/Mixtures	TDI	any mixture of TDI isomers; most commonly 80/20	26471-62-5
	80/20 TDI	a mixture of 80% 2,4-TDI and 20% 2,6-TDI	26471-62-5
	65/35 TDI	a mixture of 65% 2,4-TDI and 35% 2,6-TDI	26471-62-5
Isomers	2,4-TDI	most common isomer	584-84-9
	2,6-TDI	not commercially produced	91-08-7

### D. TDI Synonyms

TDI is identified by numerous names besides those given by the CAS and IUPAC systems. Table D lists various names for TDI which have been found in the literature. This list is not necessarily exhaustive. Also, be aware that, while each name used in a column has been used to refer to the form given in the column header, the synonym does not necessarily refer only to that type of TDI. For example “toluene diisocyanate” has been used as a synonym for generic TDI. However, “toluene diisocyanate” also may be used as a synonym for 2,4-TDI. Where the name is ambiguous, refer to the CASRN, if available, to determine the specific content of any TDI product

**Table D: TDI Synonyms**

2,4-TDI	2,6-TDI	Mixed Isomer or Non-isomer Specific
2,4-diisocyanatotoluene	2,6-diisocyanato-methylbenzene	toluene diisocyanate
2,4-diisocyanato-1-methylbenzene	2,6-diisocyanatotoluene	diisocyanatotoluene
isocyanic, 4-methyl-m-phenylene ester	isocyanic acid, 2-methyl-m-phenylene ester	isocyanic acid, methyl-m-phenylene ester
2,4-toluene diisocyanate	2,6-toluene diisocyanate	
toluene 2,4-diisocyanate	toluene 2,6-diisocyanate	
2,4-tolylene diisocyanate	2,6-tolylene diisocyanate	
tolylene 2,4-diisocyanate	tolylene 2,6-diisocyanate	
2,4-tolylene	2,6-tolylene	
tolylene 2,4-diisocyanate	tolylene 2,6-diisocyanate	
4-methyl-m-phenylene isocyanate	2-methyl-m-phenylene isocyanate	