

## 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of TDI and MDI is provided in Table 4-1.

TDI and MDI have widespread commercial use due to their reactivity and versatility. TDI and MDI and their related polyisocyanates make up >90% of the commercial market (EPA 2011a). Commercial-grade TDI is made up of an 80:20 mixture of isomers 2,4- and 2,6-TDI and represents >95% of TDI industrial use (NIOSH 1989).

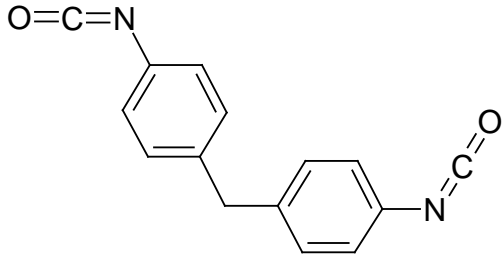
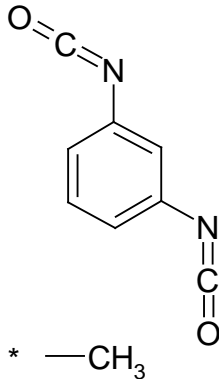
Commercial-grade MDI consists of several isomers, including 4,4'-, 2,4'-, and 2,2'-MDI, as well as oligomers and polymeric compounds. The principal commercial product of MDI is made up of a mixture of all of these components, with a typical composition in the range of 40–50% 4,4'-MDI, 2.5–4.0% 2,4'-MDI, and 0.1–0.2% 2,2'-MDI; the remainder is oligomers. 4,4'-MDI is the most commercially common isomer and is referred to as pure MDI (IARC 1999a).

### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of TDI and MDI is provided in Table 4-2.

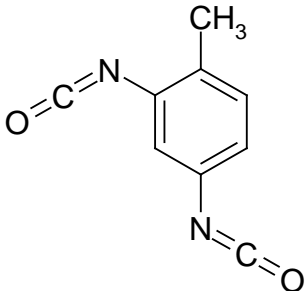
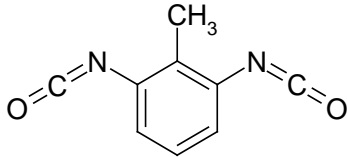
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**Table 4-1. Chemical Identity of Toluene Diisocyanate and Methylene-diphenyl Diisocyanate<sup>a</sup>**

Characteristic	Methylene-diphenyl diisocyanate	Toluene diisocyanate
Chemical name	Benzene, 1,1'-methylenebis(4-isocyanato-)	Benzene, 1,3-diisocyanato-methyl-
Synonyms(s)	4,4'-Methylenedi(phenyl isocyanate); 4,4'-methylenebis(phenyl isocyanate); 4,4'-methylene-diphenyl diisocyanate; bis(4-isocyanatophenyl)methane; isocyanic acid, methylenedi-p-phenylene ester; MDI	Diisocyanatotoluene; isocyanic acid, methylphenylene ester; methylphenylene isocyanate; TDI
Registered trade name(s)	Caradate 30; Desmodur 44; Hylene M; Isonate M; Nacconate	TDI 80/20; Mondur TD; Hylene T; Rubinate TDI; Niaux TDI
Chemical formula	C <sub>15</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
Chemical structure		
Identification numbers:		
CAS registry	101-68-8 9016-87-9 (polymeric MDI)	26471-62-5 (mixture of 2,4-TDI and 2,6-TDI)
NIOSH RTECS	NQ9350000 <sup>b</sup>	NQ9490000 <sup>e</sup>
EPA hazardous waste	No data	U223
OHM/TADS	No data	No data
DOT/UN/NA/IMCO shipping	UN 2489 <sup>c</sup> IMO 6.1 <sup>d</sup>	UN 2078 IMO 6.1
HSDB	2630	6003
NCI	C50668	No data

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**Table 4-1. Chemical Identity of Toluene Diisocyanate and Methylenediphenyl Diisocyanate<sup>a</sup>**

Characteristic	2,4-Toluene diisocyanate	2,6-Toluene diisocyanate
Chemical name	Benzene, 2,4-diisocyanato-1-methyl	Benzene, 1,3-diisocyanato-2-methyl
Synonyms(s)	2,4-Diisocyanatotoluene; isocyanic acid, 4-methyl-m-phenylene ester; 4-methyl-phenylene diisocyanate; toluene-2,4-diisocyanate; 2,4-TDI	2,6-Diisocyanatotoluene; 2,6-diisocyanato-1-methylbenzene; 2-methyl-phenylene diisocyanate; toluene-2,6-diisocyanate; 2,6-TDI
Registered trade name(s)	Hylene T; Mondur TDS	Hylene T; Mondur TDS
Chemical formula	C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
Chemical structure		
Identification numbers:		
CAS registry	584-84-9	91-08-7
NIOSH RTECS	CZ6300000 <sup>f</sup>	CZ6310000 <sup>g</sup>
EPA hazardous waste	U223	U223
OHM/TADS	No data	No data
DOT/UN/NA/IMCO shipping	UN 2206/2207/2478/3080 <sup>d</sup> IMO 6.1	UN 2207 <sup>d</sup> IMO 6.1
HSDB	874	5272
NCI	C50533	No data

<sup>a</sup>All information obtained from HSDB (2012), unless otherwise noted.

<sup>b</sup>RTECS 2009a

<sup>c</sup>ChemSpider 2013

<sup>d</sup>Lewis 2004

<sup>e</sup>NIOSH 1989

<sup>f</sup>RTECS 2009b

<sup>g</sup>RTECS 2009c

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/Intergovernmental Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS=Registry of Toxic Effects of Chemical Substances

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**Table 4-2. Physical and Chemical Properties of Toluene Diisocyanate and Methylene-diphenyl Diisocyanate<sup>a</sup>**

Property	Methylene-diphenyl diisocyanate	Toluene diisocyanate
Molecular weight	250.252	174.16
Color	Light-yellow	Clear, colorless to pale yellow
Physical state	Solid/crystals	Liquid
Melting point	37°C	11–14°C
Boiling point	196°C (at 5 mm Hg)	250°C
Density:		
at 25°C	No data	1.22 g/mL
at 70°C	1.197 g/cm <sup>3</sup>	No data
Odor	Odorless	Pungent
Odor threshold:		
Water	Not applicable <sup>b</sup>	Not applicable <sup>b</sup>
Air	No data	360–920 µg/m <sup>3</sup>
Solubility:		
Water at 25°C	Not applicable <sup>b</sup>	Not applicable <sup>b</sup>
Organic solvents	Soluble in acetone, benzene, kerosene, and nitrobenzene	Miscible with alcohol, ether, acetone, carbon tetrachloride, benzene, and kerosene
Partition coefficients:		
Log K <sub>ow</sub>	Not applicable <sup>b</sup>	Not applicable <sup>b</sup>
Log K <sub>oc</sub>	Not applicable <sup>b</sup>	Not applicable <sup>b</sup>
Vapor pressure at 25°C	5.1x10 <sup>-6</sup> mm Hg	2.30x10 <sup>-2</sup> mm Hg
Henry's law constant at 25°C	Not applicable <sup>b</sup>	Not applicable <sup>b</sup>
Autoignition temperature	No data	No data
Flashpoint	202°C (open cup)	132°C (closed cup)
Flammability limits	Flammable <sup>c</sup>	0.9–9.5 volume %
Conversion factors	1 ppm=10.24 mg/m <sup>3</sup>	No data
Explosive limits	No data	Explosive (vapor)

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**Table 4-2. Physical and Chemical Properties of Toluene Diisocyanate and Methylenediphenyl Diisocyanate<sup>a</sup>**

Property	2,4-Toluene diisocyanate	2,6-Toluene diisocyanate
Molecular weight	174.16	174.16
Color	Colorless to pale yellow	Colorless to pale yellow
Physical state	Liquid	Liquid
Melting point	20.5°C	18.3°C
Boiling point	251°C	129–133°C (at 18 mm Hg)
Density:		
at 20°C/4°C	1.2244	No data
at 25°C	No data	1.22
Odor	Sharp, pungent	Pungent
Odor threshold:		
Water	Not applicable <sup>b</sup>	Not applicable <sup>b</sup>
Air	0.4–2.14 ppm	No data
Solubility:		
Water at 25°C	Not applicable <sup>b</sup>	Not applicable <sup>b</sup>
Organic solvents	Miscible with alcohol (decomposition), ether, acetone, benzene, carbon tetrachloride, chlorobenzene, diglycol monomethyl ether, kerosene, and olive oil	Soluble in acetone and benzene
Partition coefficients:		
Log K <sub>ow</sub>	Not applicable <sup>b</sup>	Not applicable <sup>b</sup>
Log K <sub>oc</sub>	Not applicable <sup>b</sup>	Not applicable <sup>b</sup>
Vapor pressure at 25°C	8.0x10 <sup>-3</sup> mm Hg (20°C)	2.09x10 <sup>-2</sup> mm Hg
Henry's law constant at 25°C	Not applicable <sup>b</sup>	Not applicable <sup>b</sup>
Autoignition temperature	620°C	No data
Flashpoint	132°C (open cup) <sup>c</sup>	No data
Flammability limits	0.9–9.5 volume %	Flammable
Conversion factors	No data	1 mg/m <sup>3</sup> =0.14 ppm
Explosive limits	Explosive (vapor)	No data

<sup>a</sup>All information obtained from HSDB (2012), unless otherwise noted.

<sup>b</sup>Diisocyanates hydrolyze rapidly in water; therefore, these end points are not applicable.

<sup>c</sup>Lewis 2004