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 1999).

4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

Table 4-1. Chemical Identity of Toluene Diisocyanate and Methylenediphenyl Diisocyanate[a]

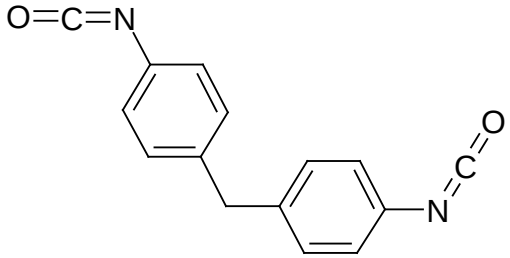
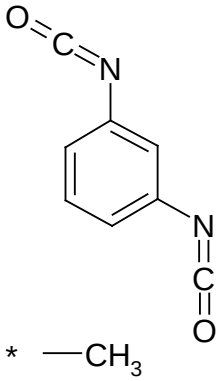
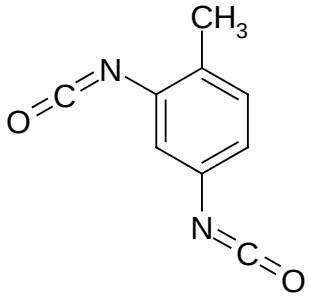
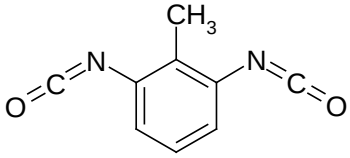
Characteristic	Methylenediphenyl diisocyanate	Toluene diisocyanate
Chemical name	Benzene, 1,1'-methylenebis(4-isocyanato-	Benzene, 1,3-diisocyanato-methyl-
Synonyms(s)	4,4'-Methylenedi(phenyl isocyanate); 4,4'-methylenediphenyl diisocyanate; bis(4-isocyanatophenyl)methane; isocyanic acid, methylenedi-p-phenylene 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; Niax TDI
Chemical formula	$C_{15}H_{10}N_2O_2$	$C_9H_6N_2O_2$
Chemical structure		
Identification numbers:		
CAS registry	101-68-8	26471-62-5
NIOSH RTECS	NQ9350000[b]	NQ9490000[e]
EPA hazardous waste	No data	U223
OHM/TADS	No data	No data
DOT/UN/NA/IMCO shipping	UN 2489[c] IMO 6.1[d]	UN 2078 IMO 6.1
HSDB	2630	6003
NCI	C50668	No data

Table 4-1. Chemical Identity of Toluene Diisocyanate and Methylenediphenyl Diisocyanate[a]

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-diisocyanto-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	$C_9H_6N_2O_2$	$C_9H_6N_2O_2$
Chemical structure		
Identification numbers:		
CAS registry	584-84-9	91-08-7
NIOSH RTECS	CZ6300000[f]	CZ6310000[g]
EPA hazardous waste	U223	U223
OHM/TADS	No data	No data
DOT/UN/NA/IMCO shipping	UN 2206/2207/2478/3080[d] IMO 6.1	UN 2207[d] IMO 6.1
HSDB	874	5272
NCI	C50533	No data

[a]All information obtained from HSDB (2012), unless otherwise noted.
[b]RTECS 2009a
[c]ChemSpider 2013
[d]Lewis 2004
[e]NIOSH 1989
[f]RTECS 2009b
[g]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

Table 4-2. Physical and Chemical Properties of Toluene Diisocyanate and Methylenediphenyl Diisocyanate[a]

Property	Methylenediphenyl 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^3	No data
Odor	Odorless	Pungent
Odor threshold:		
Water	Not applicable[b]	Not applicable[b]
Air	No data	360–920 μg/m^3
Solubility:		
Water at 25°C	Not applicable[b]	Not applicable[b]
Organic solvents	Soluble in acetone, benzene, kerosene, and nitrobenzene	Miscible with alcohol, ether, acetone, carbon tetrachloride, benzene, and kerosene
Partition coefficients:		
Log K_{ow}	Not applicable[b]	Not applicable[b]
Log K_{oc}	Not applicable[b]	Not applicable[b]
Vapor pressure at 25°C	5.1x10^{-6} mm Hg	2.30x10^{-2} mm Hg
Henry's law constant at 25°C	Not applicable[b]	Not applicable[b]
Autoignition temperature	No data	No data
Flashpoint	202°C (open cup)	132°C (closed cup)
Flammability limits	Flammable[c]	0.9–9.5 volume %
Conversion factors	1 ppm=10.24 mg/m^3	No data
Explosive limits	No data	Explosive (vapor)

Table 4-2. Physical and Chemical Properties of Toluene Diisocyanate and Methylenediphenyl Diisocyanate[a]

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[b]	Not applicable[b]
Air	0.4–2.14 ppm	No data
Solubility:		
Water at 25°C	Not applicable[b]	Not applicable[b]
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_{ow}	Not applicable[b]	Not applicable[b]
Log K_{oc}	Not applicable[b]	Not applicable[b]
Vapor pressure at 25°C	8.0×10^{-3} mm Hg (20°C)	2.09×10^{-2} mm Hg
Henry's law constant at 25°C	Not applicable[b]	Not applicable[b]
Autoignition temperature	620°C	No data
Flashpoint	132°C (open cup)[c]	No data
Flammability limits	0.9–9.5 volume %	Flammable
Conversion factors	No data	1 mg/m^3=0.14 ppm
Explosive limits	Explosive (vapor)	No data

[a]All information obtained from HSDB (2012), unless otherwise noted.
[b]Diisocyanates hydrolyze rapidly in water; therefore, these end points are not applicable.
[c]Lewis 2004