

MDI Synonyms, Acronyms, and CAS Registry Numbers

An individual MDI molecule (monomer) can exist in more than one isomeric form. Sometimes MDI is produced in a relatively pure form (usually the 4,4'-MDI isomer), sometimes it is produced as a mixture of isomers, which may be known as "generic MDI." Sometimes MDI manufactured as a monomer is further processed so that some of the MDI molecules link together to form homopolymers (dimers, trimers and oligomers); the mixture of monomers and homopolymers is called "modified MDI." In addition, a particular manufacturing process can itself produce a mixture of individual MDI molecules and homopolymers; this is known as "polymeric MDI."

At least two formal systems of nomenclature are used to describe MDI 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 (CASTM) 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 MDI and MDI 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

MDI Acronyms

MDI 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 MDI species.

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

CASRN	CA Index/Preferred Name	Short Name
101-68-8	benzene, 1,1'-methylenebis[4-isocyanato-	4,4'-MDI
5873-54-1	benzene, 1-isocyanato-2-[(4-isocyanatophenyl)methyl]-	2,4'-MDI
2536-05-2	benzene, 1,1'-methylenebis[2-isocyanato	2,2'-MDI
26447-40-5*	benzene, 1,1-methylenebis[isocyanato-*	generic MDI*
25686-28-6	benzene, 1,1'-methylenebis[4-isocyanato-, homopolymer	4,4'-MDI homopolymer
9016-87-9	isocyanic acid, polymethylenepolyphenylene ester	polymeric MDI
39310-05-9	benzene, 1,1'-methylenebis[isocyanato-, homopolymer	generic MDI homopolymer
17589-24-1	1,3-diazetidone-2,4-dione, 1,3-bis[4-[(4-isocyanatophenyl)methyl]phenyl]-	4,4'-MDI dimer
31107-36-5	1,3-diazetidone-2-one, 1,3-bis[4-[(4-isocyanatophenyl)methyl]phenyl]-4-[[4-[(4-isocyanatophenyl)methyl]phenyl]imino]-	uretonimine of 4,4'-MDI
109331-54-6**	benzene, 1,1'-methylenebis[4-isocyanato-, polymer with 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene**	4,4'-MDI/2,4'-MDI copolymer**

* For purposes of the Toxic Substances Control Act, this CASRN and name should be used for all isomeric mixtures of MDI. 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 MDI species; these names are used primarily in academic literature.

Table B: MDI IUPAC Nomenclature

Species	IUPAC Name
4,4'-MDI	1-isocyanato-4-(4-isocyanatobenzyl)benzene
2,4'-MDI	1-isocyanato-2-(4-isocyanatobenzyl)benzene
2,2'-MDI	1-isocyanato-2-(2-isocyanatobenzyl)benzene
Polymeric MDI	No name, because it is a mixture

C. MDI Acronyms

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

Table C: MDI ACRONYMS

Type	Acronym	Description/Comment	CASRN
Generic	MDI	mixture of MDI monomers	26447-40-5
Isomers	Pure MDI	4,4'-MDI	101-68-8
	2,2'-MDI	Not commercially produced	2536-05-2
	2,4'-MDI	Not commercially produced	5873-54-1
	4,4'-MDI	most common isomer	101-68-8
Polymeric	Polymeric MDI PMDI PMPI PMPPI PAPI	mixture of MDI monomers (predominantly 4,4'-MDI) & related higher molecular weight species	9016-87-9

D. MDI Synonyms

MDI is identified by numerous names besides those given by the CAS and IUPAC systems. Table C lists various names for MDI 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 MDI. For example “monomeric MDI” has been used as a synonym for 4,4'-MDI. However, “monomeric MDI” also may be used as a synonym for a mixture of monomeric MDI isomers. Similarly, the names listed under “non-isomer-specific” MDI may be applied to MDI that consists of purified 4,4'-MDI as well as to generic MDI (mixture of isomers). Where the name is ambiguous, refer to the CASRN, if available, to determine the specific content of any MDI product.

Table D: MDI Synonyms

4,4'-MDI	Generic or Non-Isomer-Specific MDI	Polymeric MDI
MDI	methylene diphenyl diisocyanate	technical MDI
pure MDI	diisocyanatodiphenylmethane	crude MDI
monomeric MDI	methylenediphenylene diisocyanate	polymethylene polyphenyl isocyanate
bis-(p-isocyanatophenyl)methane	diphenylmethane diisocyanate	polymeric diphenylmethane diisocyanate
bis-(4-isocyanatophenyl)methane	diphenyl methane diisocyanate	oligomeric MDI
di-(4-isocyanatophenyl)methane	di-(isocyanato phenyl)methane	isocyanic acid, polymethylene-polyphenylene ester
diphenylmethane-4,4'-diisocyanate	methylenebis(phenylisocyanate)	polymeric methylene diphenyl diisocyanate
isocyanic acid, methylenedi-p-phenylene ester	diphenylmethyl diisocyanate	
methylenebis(p-phenyl isocyanate)		
methylenebis(p-phenylene isocyanate)		
methylenebis(4-phenyl isocyanate)		
methylenebis(4-phenylene isocyanate)		
4,4'-diisocyanatodiphenylmethane		
4,4'-diphenylmethane diisocyanate		
4,4'-methylenebis(phenyl isocyanate)		
4,4'-methylenediphenyl diisocyanate		
4,4'-methylenediphenylene isocyanate		