



SAFETY DATA SHEET

Version 6.13 Revision Date 01/02/2025 Print Date 01/03/2025

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Tolylene-2,4-diisocyanate

Product Number : 216836

Brand : Aldrich

Index-No. : 615-006-00-4

CAS-No. : 584-84-9

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption

(40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by

MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.

3050 SPRUCE ST ST. LOUIS MO 63103 UNITED STATES

Telephone : +1 314 771-5765 Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-

527-3887 CHEMTREC (International) 24

Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute toxicity : Category 1

(Inhalation)

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Skin irritation : Category 2

Eye irritation : Category 2A

Respiratory sensitization : Category 1

Skin sensitization : Category 1

Carcinogenicity : Category 2

icity - single exposure

Specific target organ tox- : Category 3 (Respiratory system)

Short-term (acute) aquatic hazard

: Category 3

Long-term (chronic)

aquatic hazard

: Category 3

GHS label elements

Hazard pictograms







Signal Word Danger

Hazard Statements : H315 Causes skin irritation.

H317 May cause an allergic skin reaction.

H319 Causes serious eye irritation.

H330 Fatal if inhaled.

H334 May cause allergy or asthma symptoms or

breathing difficulties if inhaled.

H335 May cause respiratory irritation. H351 Suspected of causing cancer.

H412 Harmful to aquatic life with long lasting effects.

Precautionary Statements: **Prevention:**

P201 Obtain special instructions before use.

P202 Do not handle until all safety precautions have

been read and understood.

P260 Do not breathe mist or vapors.

P264 Wash skin thoroughly after handling.

P271 Use only outdoors or in a well-ventilated area. P272 Contaminated work clothing must not be allowed

out of the workplace.

P273 Avoid release to the environment.

P280 Wear protective gloves/ protective clothing/ eye

protection/ face protection.

P284 Wear respiratory protection.

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Response:

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

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

P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.

P337 + P313 If eye irritation persists: Get medical advice/ attention.

P342 + P311 If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.

P362 Take off contaminated clothing and wash before reuse.

Storage:

P403 + P233 Store in a well-ventilated place. Keep container tightly closed. P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

Other hazards

None known.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Chemical name	CAS-No.	Concentration (% w/w)
4-methyl-m-phenylene diisocya-	584-84-9	>= 90 - <= 100
nate		

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : First aiders need to protect themselves.

Show this material safety data sheet to the doctor in

attendance.

If inhaled : After inhalation: fresh air. Immediately call in physi-

cian.

If breathing stops: immediately apply artificial respira-

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tion, if necessary also oxygen.

In case of skin contact : In case of skin contact: Take off immediately all con-

taminated clothing. Rinse skin with water/ shower.

Consult a physician.

In case of eye contact : After eye contact: rinse out with plenty of water.

Call in ophthalmologist. Remove contact lenses.

If swallowed : After swallowing: immediately make victim drink wa-

ter (two glasses at most).

Consult a physician.

Most important symptoms and effects, both acute and delayed

: The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in

section 11

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

SECTION 5. FIRE-FIGHTING MEASURES

Suitable extinguishing

media

: Water Foam

Carbon dioxide (CO2)

Dry powder

Unsuitable extinguishing

media

For this substance/mixture no limitations of extin-

guishing agents are given.

Specific hazards during

fire fighting

: Combustible.

Vapors are heavier than air and may spread along

floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or va-

pours possible in the event of fire.

Hazardous combustion

products

: Carbon oxides

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Nitrogen oxides (NOx)

Specific extinguishing

methods

: No data available

Further information : Suppress (knock down) gases/vapors/mists with a

water spray jet.

Prevent fire extinguishing water from contaminating

surface water or the ground water system.

Special protective equip-

ment for fire-fighters

Stay in danger area only with self-contained breathing

apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:

Do not breathe vapors, aerosols.

Avoid substance contact.
Ensure adequate ventilation.

Evacuate the danger area, observe emergency proce-

dures, consult an expert.

Advice for emergency responders: For personal protection see section 8.

Environmental precau-

tions

: Do not let product enter drains.

Methods and materials for containment and

cleaning up

: Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7

and 10).

Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected

area

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on safe handling : Work under hood. Do not inhale substance/mixture.

Avoid generation of vapours/aerosols.

Further information on storage conditions

: Tightly closed.

Keep in a well-ventilated place.

Keep locked up or in an area accessible only to quali-

fied or authorized persons.

Storage class : 6.1A, Combustible, acute toxic Cat. 1 and 2 / very

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toxic hazardous materials

Recommended storage

temperature

: 36 - 46 °F / 2 - 8 °C

Further information on

storage stability

: Store under inert gas.

Product is sensitive to light and moisture.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
4-methyl-m-phenylene diisocyanate	584-84-9	TWA	0.0050 ppm	ACGIH
		STEL	0.02 ppm	ACGIH
		С	0.02 ppm 0.14 mg/m3	OSHA Z-1
		TWA	0.0050 ppm 0.04 mg/m3	OSHA P0
		STEL	0.02 ppm 0.15 mg/m3	OSHA P0

Biological occupational exposure limits

Components	CAS-No.	Control parame-	Biological specimen	Sam- pling	Permissi- ble con-	Basis
		ters		time	centration	
4-methyl-m- phenylene diisocya- nate	584-84-9	toluene diamine	Urine	End of shift	5 μg/g creatinine	ACGIH BEI

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter

type:

: Filter type ABEK

The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly

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documented.

Hand protection

Remarks : required

Eye protection : Use equipment for eye protection tested and ap-

proved under appropriate government standards such

as NIOSH (US) or EN 166(EU).

Safety glasses

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply

preventive skin protection. Wash hands and face af-

ter working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : clear, liquid

Color : colorless

Odor : No data available

Odor Threshold : No data available pH : No data available

Melting point/ range : 68 - 72 °F / 20 - 22 °C

Method: lit.

Boiling point/boiling range : 239 - 248 °F / 115 - 120 °C

(13 hPa) Method: lit.

Flash point : 270 °F / 132 °C

Method: closed cup

Evaporation rate : No data available

Burning rate : No data available

Upper explosion limit / Upper flammability limit

: 9.5 %(V)

Lower explosion limit / Lower flammability limit : 0.9 %(V)

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Vapor pressure : 0.04 hPa (77 °F / 25 °C)

Relative vapor density : 6.01

(Air = 1.0)

Relative density : 1.21 (77 °F / 25 °C)

Method: Regulation (EC) No. 440/2008, Annex, A.3

GLP: yes

Density : 1.225 g/cm3 (77 °F / 25 °C)

Water solubility : No data available

Partition coefficient: n-

octanol/water

: log Pow: 3.43 (72 °F / 22 °C)

pH: 7

Method: OECD Test Guideline 117 Bioaccumulation is not expected.

Autoignition temperature : > 1148 °F / > 620 °C

Decomposition tempera-

ture

: No data available

Viscosity, dynamic : No data available

Viscosity, kinematic : No data available

Flow time : No data available

Explosive properties : Method: Explosive properties

GLP: yes

Not classified as explosive.

Oxidizing properties : none

Surface tension : 25 mN/m, 77 °F / 25 °C

Molecular weight : 174.16 g/mol

Particle characteristics

Particle size : No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity : Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point

is to be rated as critical.

Chemical stability : The product is chemically stable under standard ambi-

ent conditions (room temperature).

Possibility of hazardous

reactions

: No data available

Conditions to avoid : Heat.

Strong heating.

Incompatible materials : Alcohols

> Strong bases **Amines** acids

Strong oxidizing agents

products

Hazardous decomposition: In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male - 5,110 mg/kg

(OECD Test Guideline 401)

Remarks: (in analogy to similar compounds)

The value is given in analogy to the following substances: m-tolylidene diisocya-

nate

LC50 Inhalation - Rat - male and female - 4 h - 0.12 mg/l - vapor

(OECD Test Guideline 403)

Remarks: (in analogy to similar products) Inhalation: Irritating to respiratory system.

LD50 Dermal - Rabbit - male and female - > 9,400 mg/kg

(OECD Test Guideline 402)

Remarks: (in analogy to similar products)

The value is given in analogy to the following substances: m-tolylidene diisocya-

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h

Remarks: (RTECS)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table

3.1/3.2)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes.

(Draize Test) Remarks: (ECHA)

Aldrich- 216836 Page 9 of 17 Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

Open epicutaneous test - Guinea pig

Result: positive Remarks: (ECHA)

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2) May cause allergy or asthma symptoms or breathing difficulties if inhaled. Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Germ cell mutagenicity

Test Type: Ames test

Test system: S. typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: positive

Test Type: In vivo micronucleus test

Species: Rat

Application Route: Inhalation

Method: Mutagenicity (micronucleus test)

Result: negative

Test Type: unscheduled DNA synthesis assay

Species: Rat

Application Route: Inhalation

Result: negative Remarks: (ECHA)

Test Type: Micronucleus test

Species: Mouse

Application Route: Inhalation Method: OECD Test Guideline 474

Result: negative

Carcinogenicity

Suspected of causing cancer.

IARC: 2B - Group 2B: Possibly carcinogenic to humans (4-methyl-m-phenylene

diisocyanate)

NTP: RAHC - Reasonably anticipated to be a human carcinogen (4-methyl-m-

phenylene diisocyanate)

OSHA: No component of this product present at levels greater than or equal to

0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Respiratory Tract

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

RTECS: CZ6300000

Cough, Shortness of breath, Headache, Nausea, Vomiting

To the best of our knowledge, the chemical, physical, and toxicological properties

have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

4-methyl-m-phenylene diisocyanate:

Toxicity to fish : LC50 (Oncorhynchus mykiss (rainbow trout)): 133

mg/l

Exposure time: 96 h
Test Type: static test
Analytical monitoring: yes

Method: OECD Test Guideline 203

Remarks: (in analogy to similar products)

Toxicity to daphnia and

other aquatic inverte-

brates

: EC50 (Daphnia magna (Water flea)): 12.5 mg/l

Exposure time: 48 h Test Type: static test Analytical monitoring: yes

Method: OECD Test Guideline 202

Remarks: (in analogy to similar products)

Toxicity to algae/aquatic

plants

EC50 (Skeletonema costatum (marine diatom)):

3,230 mg/l

Exposure time: 96 h Analytical monitoring: yes

Method: OECD Test Guideline 201

Remarks: (in analogy to similar products)

Toxicity to daphnia and

other aquatic inverte-

: EC50 (Daphnia magna (Water flea)): 2 mg/l

End point: reproduction rate

brates (Chronic toxicity) Exposure time: 21 d

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Test Type: static test Analytical monitoring: yes

Method: OECD Test Guideline 211

GLP: yes

Remarks: (in analogy to similar products)

Toxicity to microorgan-

isms

: EC50 (activated sludge): > 100 mg/l

Exposure time: 3 h

Method: OECD Test Guideline 209

Remarks: (in analogy to similar products)

Persistence and degradability

Components:

4-methyl-m-phenylene diisocyanate:

Biodegradability : aerobic

Inoculum: activated sludge Concentration: 30 mg/l Biochemical oxygen demand Result: Not biodegradable Biodegradation: 0 % Exposure time: 28 d

Method: OECD Test Guideline 302C

Remarks: (in analogy to similar compounds)

Bioaccumulative potential

Components:

4-methyl-m-phenylene diisocyanate:

Bioaccumulation : Species: Cyprinus carpio (Carp)

Bioconcentration factor (BCF): 180

Exposure time: 60 d

Temperature: 76.6 °F / 24.8 °C Concentration: 0.8 mg/l

Method: OECD Test Guideline 305

GLP: yes

Partition coefficient: n-

octanol/water

: log Pow: 3.43 (72 °F / 22 °C)

pH: 7

Method: OECD Test Guideline 117

Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Product:

Ozone-Depletion Potential: Regulation: 40 CFR Protection of Environment; Part 82

Protection of Stratospheric Ozone - CAA Section 602

Class I Substances

Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR

82, Subpt. A, App.A + B).

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance

with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product

itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 2078

Proper shipping name : Toluene diisocyanate

Class : 6.1 Packing group : II

Labels : Division 6.1 - Toxic substances

Packing instruction (cargo: 662

aircraft)

Packing instruction (pas- : 654

senger aircraft)

IMDG-Code

UN number : UN 2078

Proper shipping name : TOLUENE DIISOCYANATE

Class : 6.1
Packing group : II
Labels : 6.1
EmS Code : F-A, S-A
Marine pollutant : no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National regulation

49 CFR Road

UN/ID/NA number : UN 2078

Proper shipping name : Toluene diisocyanate

Class : 6.1 Packing group : II

Labels : Division 6.1 - Toxic substances

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ERG Code : 156 Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

Components	CAS-No.	Component RO (lbs)	Calculated product RO (lbs)
4-methyl-m-phenylene diiso-	584-84-9	100	100
cyanate			

SARA 304 Extremely Hazardous Substances Reportable Quantity

Components	CAS-No.	Component RO (lbs)	Calculated product RQ (lbs)
4-methyl-m-phenylene diiso-	584-84-9	100	100
cyanate			

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

Components	CAS-No.	Component TPQ (lbs)
4-methyl-m-phenylene diiso-	584-84-9	500
cvanate		

SARA 311/312 Hazards
: Acute Health Hazard
Chronic Health Hazard

SARA 313 : The following components are subject to reporting

levels established by SARA Title III, Section 313:

4-methyl-m- 584-84-9 >= 90 - <= 100 %

phenylene diisocyanate

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B). The following chemical(s) are listed as HAP under the U.S. Clean Air Act, Section 112 (40 CFR 61):

4-methyl-m- 584-84-9 >= 90 - <= 100 % phenylene diisocya-

nate

пасе

The following chemical(s) are listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F):

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4-methyl-m- 584-84-9 >= 90 - <= 100 % phenylene diisocya- nate

The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCMI Intermediate or Final VOC's (40 CFR 60.489):

4-methyl-m- 584-84-9 >= 90 - <= 100 % phenylene diisocya- nate

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. Clean-Water Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

4-methyl-m-phenylene diisocyanate 584-84-9

Pennsylvania Right To Know

4-methyl-m-phenylene diisocyanate 584-84-9

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

The following substance(s) is/are subject to a Significant New Use Rule: 4-methyl-m-phenylene diisocy- 584-84-9 Proposed Rule anate

The following substance(s) is/are subject to TSCA 12(b) export notification requirements:

4-methyl-m-phenylene diisocy- 584-84-9 anate

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SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH : USA. ACGIH Threshold Limit Values (TLV)
ACGIH BEI : ACGIH - Biological Exposure Indices (BEI)

OSHA PO : USA. Table Z-1-A Limits for Air Contaminants (1989)

vacated values)

OSHA Z-1 : USA. Occupational Exposure Limits (OSHA) - Table Z-

1 Limits for Air Contaminants

ACGIH / TWA : 8-hour, time-weighted average ACGIH / STEL : Short-term exposure limit : 8-hour time weighted average OSHA PO / STEL : Short-term exposure limit

OSHA Z-1 / C : Ceiling

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT -Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA -Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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Revision Date : 01/02/2025

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