

SAFETY DATA SHEET

1. PRODUCT

1.1 Product identifiers

Name: 1,3-Bis(1-isocyanato-1-methylethyl)benzene

CAS-No.: 2778-42-9

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

Identified uses : Laboratory chemicals, Manufacture of substances

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Inhalation (Category 1), H330

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

Skin sensitisation (Category 1), H317


Specific target organ toxicity - repeated exposure, Inhalation (Category 1), Lungs, H372

Acute aquatic toxicity (Category 1), H400

Chronic aquatic toxicity (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram	
Signal word	Danger
Hazard statement(s)	H315 Causes skin irritation. H317 May cause an allergic skin reaction. H319 Causes serious eye irritation. H330 Fatal if inhaled. H372 Causes damage to organs (Lungs) through prolonged or repeated exposure if inhaled. H410 Very toxic to aquatic life with long lasting effects.
Precautionary statement(s)	P260 Do not breathe dust/ fume/ gas/ mist/ vapours/ spray. P264 Wash skin thoroughly after handling. P270 Do not eat, drink or smoke when using this product. P271 Use only outdoors or in a well-ventilated area. P272 Contaminated work clothing should not be allowed out of the workplace. P273 Avoid release to the environment. P280 Wear protective gloves/ eye protection/ face protection. P284 Wear respiratory protection. P302 + P352 IF ON SKIN: Wash with plenty of soap and water. P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P310 Immediately call a POISON CENTER or doctor/ physician. P320 Specific treatment is urgent (see supplemental first aid instructions on this label). P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention. P337 + P313 If eye irritation persists: Get medical advice/ attention. P362 Take off contaminated clothing and wash before reuse. P391 Collect spillage. P403 + P233 Store in a well-ventilated place. Keep container tightly closed. P405 Store locked up. P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Lachrymator.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms: ,,,-Tetramethyl-1,3-xylylene diisocyanate
Formula: C₁₄H₁₆N₂O₂
Molecular weight: 244.29 g/mol
CAS-No.: 2778-42-9
EC-No.: 220-474-4

Hazardous components

Component	Classification	Concentration
1,3-Bis(1-isocyanato-1-methylethyl)benzene		
	Acute Tox. 1; Skin Irrit. 2; Eye Irrit. 2A; Skin Sens. 1; STOT RE 1; Aquatic Acute 1; Aquatic Chronic 1; H315, H317, H319, H330, H372, H410	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.
In case of skin contact
Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.
In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.
If swallowed
Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 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

4.2 Indication of any immediate medical attention and special treatment needed

No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NO_x)

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Moisture sensitive.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection	Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
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Skin protection	Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. Splash contact Material: Nitrile rubber Minimum layer thickness: 0.4 mm Break through time: 60 min Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M) data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374 If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.
Body Protection	Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.
Respiratory protection	Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).
Control of environmental exposure	Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

Appearance	Form: liquid Colour: colourless
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	4 °C (39 °F) at 101.3 hPa (76.0 mmHg) - OECD Test Guideline 102
Initial boiling point and boiling range	106 °C (223 °F) at 1.2 hPa (0.9 mmHg) - lit.
Flash point	168 °C (334 °F) - closed cup - ASTM D 56
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	0.386 hPa (0.290 mmHg) at 25 °C (77 °F)
Vapour density	No data available
Relative density	1.06 g/cm ³ at 25 °C (77 °F)
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
Auto-ignition temperature	498 °C (928 °F) at 101.3 hPa (76.0 mmHg)
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

9.2 Other safety information

Surface tension: 38.6 mN/m at 20 °C (68 °F)

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Avoid moisture.

10.5 Incompatible materials

acids, Peroxides, Alcohols, Amines, Bases

10.6 Hazardous decomposition products

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity LD50 Oral - Rat - 5,337 mg/kg (OECD Test Guideline 401) LC50 Inhalation - Rat - female - 4 h - 0.027 mg/l (OECD Test Guideline 403) LD50 Dermal - Rabbit - > 2,000 mg/kg (OECD Test Guideline 402) No data available
Skin corrosion/irritation Skin - Rabbit Result: Moderate skin irritation (OECD Test Guideline 404)
Serious eye damage/eye irritation Eyes - Rabbit Result: Eye irritation (OECD Test Guideline 405)
Respiratory or skin sensitisation Buehler Test - Guinea pig May cause allergic skin reaction.
Germ cell mutagenicity in vitro assay S. typhimurium Result: negative
Carcinogenicity IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC. ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH. NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP. OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
Reproductive toxicity No data available No data available
Specific target organ toxicity -single exposure No data available
Specific target organ toxicity -repeated exposure Inhalation - Causes damage to organs through prolonged or repeated exposure. - Lungs
Aspiration hazard No data available
Additional Information RTECS: CY8480000 burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	static test LC50 - Pimephales promelas (fathead minnow) - 0.67 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates	static test LC50 - Daphnia magna (Water flea) - 5.2 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test EC50 - Pseudokirchneriella subcapitata (green algae) - 6.9 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	No data available

12.2 Persistence and degradability

Biodegradability	Result: 13.7 % - According to the results of tests of biodegradability this product is not readily biodegradable. (Closed Bottle test)
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12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Very toxic to aquatic life with long lasting effects.

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.
Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 3382 Class: 6.1 Packing group: I

Proper shipping name: Toxic by inhalation liquid, n.o.s. (1,3-Bis(1-isocyanato-1-methylethyl)benzene)

Reportable Quantity (RQ):

Poison Inhalation Hazard: Hazard zone B

IMDG

UN number: 3382 Class: 6.1 Packing group: I EMS-No: F-A, S-A

Proper shipping name: TOXIC BY INHALATION LIQUID, N.O.S. (1,3-Bis(1-isocyanato-1-methylethyl)benzene)

Marine pollutant:yes

IATA

UN number: 3382 Class: 6.1

Proper shipping name: Toxic by inhalation liquid, n.o.s. (1,3-Bis(1-isocyanato-1-methylethyl)benzene)

IATA Passenger: Not permitted for transport

IATA Cargo: Not permitted for transport

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

Component	CAS-No.	Revision Date
1,3-Bis(1-isocyanato-1-methylethyl)benzene	2778-42-9	

New Jersey Right To Know Components

Component	CAS-No.	Revision Date
1,3-Bis(1-isocyanato-1-methylethyl)benzene	2778-42-9	

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox. Acute toxicity

Aquatic Acute Acute aquatic toxicity

Aquatic Chronic Chronic aquatic toxicity

Eye Irrit. Eye irritation

H315 Causes skin irritation.

H317 May cause an allergic skin reaction.

H319 Causes serious eye irritation.

H330 Fatal if inhaled.

H372 Causes damage to organs through prolonged or repeated exposure if inhaled.

H400 Very toxic to aquatic life.

H410 Very toxic to aquatic life with long lasting effects.

HMIS Rating

Health hazard: 4

Chronic Health Hazard:

Flammability: 1

Physical Hazard 0

NFPA Rating

Health hazard: 4

Fire Hazard: 1

Reactivity Hazard: 0
