

SAFETY DATA SHEET

Version 5.5
Revision Date 12/11/2014
Print Date 06/28/2019

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : 1,3-Bis(1-isocyanato-1-methylethyl)benzene

Product Number : 409502

Brand : Aldrich

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

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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	:	$\alpha,\alpha,\alpha',\alpha'$ -Tetramethyl-1,3-xylylene diisocyanate
Formula	:	C ₁₄ H ₁₆ N ₂ O ₂
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

4.3 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).

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

- | | |
|---|---|
| a) Appearance | Form: liquid
Colour: colourless |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | 4 °C (39 °F) at 101.3 hPa (76.0 mmHg) - OECD Test Guideline 102 |
| f) Initial boiling point and boiling range | 106 °C (223 °F) at 1.2 hPa (0.9 mmHg) - lit. |
| g) Flash point | 168 °C (334 °F) - closed cup - ASTM D 56 |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapour pressure | 0.386 hPa (0.290 mmHg) at 25 °C (77 °F) |
| l) Vapour density | No data available |
| m) Relative density | 1.06 g/cm ³ at 25 °C (77 °F) |

n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Auto-ignition temperature	498 °C (928 °F) at 101.3 hPa (76.0 mmHg)
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information

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

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)

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

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

New Jersey Right To Know Components

	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

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 5.5

Revision Date: 12/11/2014

Print Date: 06/28/2019