

SAFETY DATA SHEET

Version 6.14
Revision Date 09/09/2024
Print Date 09/10/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : *p*-Xylene-d₁₀

Product Number : 175927
Brand : Aldrich
CAS-No. : 41051-88-1

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**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
Skin irritation (Category 2), H315

Aldrich - 175927

Page 1 of 13

Eye irritation (Category 2A), H319
 Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
 Aspiration hazard (Category 1), H304
 Short-term (acute) aquatic hazard (Category 2), H401
 Long-term (chronic) aquatic hazard (Category 3), H412

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 Statements

H226	Flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H312 + H332	Harmful in contact with skin or if inhaled.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H401	Toxic to aquatic life.
H412	Harmful to aquatic life with long lasting effects.

Precautionary Statements

P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing mist or vapors.
P264	Wash skin thoroughly after handling.
P271	Use only outdoors or in a well-ventilated area.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P331	Do NOT induce vomiting.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.

P405
P501

Store locked up.
Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : 1,4-Dimethylbenzene-d10

Formula : C₈D₁₀
Molecular weight : 116.25 g/mol
CAS-No. : 41051-88-1
EC-No. : 255-193-6

Component	Classification	Concentration
<I>p</>-Xylene-d<SB>10</>		
	Flam. Liq. 3; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 3; H226, H332, H312, H315, H319, H335, H304, H401, H412	<= 100 %

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

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated 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: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂) Foam Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 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.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
p-Xylene-d10	41051-88-1	TWA	100 ppm 435 mg/m ³	USA. NIOSH Recommended Exposure Limits
		ST	150 ppm 655 mg/m ³	USA. NIOSH Recommended Exposure Limits
		TWA	100 ppm 435 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Ototoxicant Not classifiable as a human carcinogen		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
-----------	---------	------------	-------	---------------------	-------

p-Xylene-d10	41051-88-1	Methylhippuric acids	0.3g/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur 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 documented.

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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	135 °C 275 °F - lit.
g) Flash point	25.00 °C (77.00 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 7 %(V) Lower explosion limit: 1.1 %(V)
k) Vapor pressure	21 hPa at 37.70 °C (99.86 °F) 10 hPa at 20.00 °C(68.00 °F)
l) Vapor density	No data available
m) Density	0.948 g/mL at 25 °C (77 °F) - lit.0.948 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Strong oxidizing agents

conc. sulfuric acid

Nitric acid

uranium hexafluoride

sulfur

rubber

various plastics

Risk of explosion with:

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

No data available

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male - 3,523 mg/kg

(EC Directive 92/69/EEC B.1 Acute Toxicity (Oral))

Acute toxicity estimate Inhalation - 4 h - 10.1 mg/l - vapor

(Expert judgment)

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

Acute toxicity estimate Dermal - 1,000.1 mg/kg

(Expert judgment)

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

Skin corrosion/irritation

Skin - Rabbit

Result: Moderate skin irritation - 4 h

(Regulation (EC) No. 440/2008, Annex, B.4)

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

Remarks: Drying-out effect resulting in rough and chapped skin.

Dermatitis

Serious eye damage/eye irritation

Remarks: Causes serious eye irritation.
(ECHA)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: (National Toxicology Program)

Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: Regulation (EC) No. 440/2008, Annex, B.19

Result: negative

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: Mutagenicity (in vitro mammalian cytogenetic test)

Result: negative

Test Type: Mutagenicity (mammal cell test): micronucleus.

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Intraperitoneal

Method: OECD Test Guideline 474

Result: negative

Remarks: (IUCLID)

Test Type: dominant lethal test

Species: Mouse

Application Route: Subcutaneous

Method: OECD Test Guideline 478

Result: negative

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient 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 on OSHA's list of regulated carcinogens.

Reproductive toxicity

May cause reproductive disorders.

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Respiratory Tract

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

May be fatal if swallowed and enters airways.

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 90 Days - NOAEL (No observed adverse effect level) - 200 mg/kg

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish	static test LC50 - Oncorhynchus mykiss (rainbow trout) - 2.60 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 35.50 - 63.10 mg/l - 48 h Remarks: (ECOTOX Database)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata - 4.36 mg/l - 73 h (OECD Test Guideline 201)
Toxicity to bacteria	static test NOEC - activated sludge - 16.2 mg/l - 28 h Remarks: (ECHA)
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Danio rerio (zebra fish) - 0.71 mg/l - 35 d (OECD Test Guideline 210)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	static test EC50 - Daphnia magna (Water flea) - 2.9 mg/l - 21 d (OECD Test Guideline 211)
	static test NOEC - Daphnia magna (Water flea) - 1.57 mg/l - 21 d (OECD Test Guideline 211)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 98 % - Readily biodegradable.
(OECD Test Guideline 301F)

12.3 Bioaccumulative potential

Bioaccumulation Oncorhynchus mykiss (rainbow trout) - 56 d
at 10 °C - 1.3 mg/l(p-Xylene-d10)

Bioconcentration factor (BCF): 7.4 - 18.5

Aldrich - 175927

Page 10 of 13

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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

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

DOT (US)

UN number: 1307 Class: 3 Packing group: III
Proper shipping name: Xylenes
Reportable Quantity (RQ): 100 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 1307 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: XYLENES

IATA

UN number: 1307 Class: 3 Packing group: III
Proper shipping name: Xylenes

SECTION 15: Regulatory information

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
p-Xylene-d ₁₀	41051-88-1	100	100

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

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

SARA 313 : The following components are subject to reporting levels established by SARA Title III, Section 313:

<i>p</i> -Xylene-d ₁₀	41051-88-1	>= 90 - <= 100 %
----------------------------------	------------	------------------

US State Regulations**Massachusetts Right To Know**

<i>p</i> -Xylene-d ₁₀	41051-88-1
----------------------------------	------------

Pennsylvania Right To Know

<i>p</i> -Xylene-d ₁₀	41051-88-1
----------------------------------	------------

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 : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

Details in analogy to the undeuterated compound.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 6.14

Revision Date: 09/09/2024

Print Date: 09/10/2024