

SAFETY DATA SHEET

Version 6.5
Revision Date 09/21/2021
Print Date 06/02/2022

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

Product name : Styrene-2,3,4,5,6-d₅

Product Number : 589543
Brand : Aldrich
Index-No. : 601-026-00-0
CAS-No. : 5161-29-5

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

Identified uses : Laboratory chemicals, Synthesis of substances

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
Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319
Carcinogenicity (Category 1B), H350
Reproductive toxicity (Category 2), H361
Specific target organ toxicity - repeated exposure (Category 1), H372
Short-term (acute) aquatic hazard (Category 2), H401

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)

H226	Flammable liquid and vapor.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H350	May cause cancer.
H361	Suspected of damaging fertility or the unborn child.
H372	Causes damage to organs through prolonged or repeated exposure.
H401	Toxic to aquatic life.

Precautionary statement(s)

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
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.
P260	Do not breathe dust/ fume/ gas/ mist/ vapors/ 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.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
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.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
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 + P235	Store in a well-ventilated place. Keep cool.
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.

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula : C₈D₅H₃
Molecular weight : 109.08 g/mol
CAS-No. : 5161-29-5
Index-No. : 601-026-00-0

Component	Classification	Concentration
Styrene-2,3,4,5,6-d5		
	Flam. Liq. 3; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; Carc. 1B; Repr. 2; STOT RE 1; Aquatic Acute 2; H226, H332, H315, H319, H350, H361, H372, H401	<= 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. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

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: immediately make victim drink water (two glasses at most). 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Foam Carbon dioxide (CO₂) 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. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability

Recommended storage temperature
2 - 8 °C

Light sensitive.

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
Styrene-2,3,4,5,6-d5	5161-29-5	TWA	50 ppm 215 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	100 ppm 425 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	100 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		CEIL	200 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Peak	600 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		TWA	50 ppm 215 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	100 ppm 425 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		PEL	50 ppm 215 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
	Remarks	Skin		

		STEL	100 ppm 425 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		C	500 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		TWA	10 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Ototoxicant Confirmed animal carcinogen with unknown relevance to humans		
		STEL	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Ototoxicant Confirmed animal carcinogen with unknown relevance to humans		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Styrene-2,3,4,5,6-d5	5161-29-5	Mandelic acid plus phenylglyoxylic acid	400mg/g Creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			
		Styrene	40 µg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
		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

required

Body Protection

Flame retardant antistatic protective clothing.

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.

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: clear, liquid Color: colorless
b) Odor	sweet
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Freezing point: ca.-31.0 °C (ca.-23.8 °F)
f) Initial boiling point and boiling range	145 - 146 °C 293 - 295 °F - lit.
g) Flash point	ca.32 °C (90 °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: ca.8.9 %(V) Lower explosion limit: ca.1.1 %(V)
k) Vapor pressure	ca.6 hPa at ca.20 °C (ca.68 °F)
l) Vapor density	ca.3.6
m) Density	0.952 g/mL at 25 °C (77 °F) - lit.0.952 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	ca.0.05 g/l at ca.25 °C (ca.77 °F) - slightly soluble
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	ca.490.0 °C (ca.914.0 °F)
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

Relative vapor density	ca.3.6
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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) .
Stable

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

IARC: 2A - Group 2A: Probably carcinogenic to humans (Styrene-2,3,4,5,6-d5)

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

No data available

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Dermatitis, Central nervous system depression, Nausea, Dizziness, Headache

SECTION 12: Ecological information**12.1 Toxicity**

No data available

12.2 Persistence and degradability

No data available

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

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information**DOT (US)**

UN number: 2055 Class: 3 Packing group: III
Proper shipping name: Styrene monomer, stabilized
Reportable Quantity (RQ): 1000 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 2055 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: STYRENE MONOMER, STABILIZED

IATA

Aldrich - 589543

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SECTION 15: Regulatory information

SARA 302 Components

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

SARA 313 Components

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

	CAS-No.	Revision Date
Styrene-2,3,4,5,6-d5	5161-29-5	2007-07-01

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

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

SECTION 16: Other information

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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.

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Details in analogy to the undeuterated compound.

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