

SAFETY DATA SHEET

Version 7.7
Revision Date 09/06/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : *N*-[3-(Trimethoxysilyl)propyl]aniline

Product Number : 440809

Brand : Aldrich

CAS-No. : 3068-76-6

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)

Skin corrosion (Category 1B), H314

Serious eye damage (Category 1), H318

Skin sensitization (Category 1), H317

Germ cell mutagenicity (Category 2), H341

Carcinogenicity (Category 2), H351

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

Short-term (acute) aquatic hazard (Category 3), H402

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

H314

Causes severe skin burns and eye damage.

H317

May cause an allergic skin reaction.

H341

Suspected of causing genetic defects.

H351

Suspected of causing cancer.

H372

Causes damage to organs (Blood) through prolonged or repeated exposure.

H412

Harmful to aquatic life with long lasting effects.

Precautionary Statements

P201

Obtain special instructions before use.

P202

Do not handle until all safety precautions have been read and understood.

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.

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.

P301 + P330 + P331

IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P303 + P361 + P353

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.

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.

P310

Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.

P308 + P313

IF exposed or concerned: Get medical advice/ attention.

P333 + P313

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

P363

Wash contaminated clothing before reuse.

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 - none

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Formula : C₁₂H₂₁NO₃Si
Molecular weight : 255.39 g/mol

Component	Classification	Concentration
N-[3-(Trimethoxysilyl)propyl]aniline		
CAS-No. EC-No.	3068-76-6 221-328-2	Skin Corr. 1B; Eye Dam. 1; H314, H318 <= 100 %
Aniline		
CAS-No. EC-No. Index-No.	62-53-3 200-539-3 612-008-00-7	Flam. Liq. 4; Acute Tox. 3; Eye Dam. 1; Skin Sens. 1; Muta. 2; Carc. 2; STOT RE 1; Aquatic Acute 1; Aquatic Chronic 1; H227, H301, H331, H311, H318, H317, H341, H351, H372, H400, H410 Concentration limits: >= 1 %: STOT RE 1, H372; 0.2 - < 1 %: STOT RE 2, H373; M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1 >= 1 - < 5 %
Methanol		
CAS-No. EC-No. Index-No. Registration number	67-56-1 200-659-6 603-001-00-X 01-2119433307-44-XXXX	Flam. Liq. 2; Acute Tox. 3; STOT SE 1; H225, H301, H331, H311, H370 Concentration limits: >= 10 %: STOT SE 1, H370; 3 - < 10 %: STOT SE 2, H371; >= 0.1 - < 1 %

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

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

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**

Water 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

Nitrogen oxides (NO_x)

silicon oxides

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 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

Suppress (knock down) gases/vapors/mists with a water spray jet. 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. 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.

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.

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

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Light sensitive. Store under inert gas.

Storage class

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

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
Aniline	62-53-3	TWA	2 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		

		PEL	2 ppm 7.6 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)	
		Skin			
		TWA	5 ppm 19 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants	
		Skin designation			
		Potential Occupational Carcinogen			
Methanol	67-56-1	TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)	
		Danger of cutaneous absorption			
		STEL	250 ppm	USA. ACGIH Threshold Limit Values (TLV)	
		Danger of cutaneous absorption			
		ST	250 ppm 325 mg/m ³	USA. NIOSH Recommended Exposure Limits	
		Potential for dermal absorption			
		TWA	200 ppm 260 mg/m ³	USA. NIOSH Recommended Exposure Limits	
		Potential for dermal absorption			
		TWA	200 ppm 260 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants	
		PEL	200 ppm 260 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)	
		Skin			
		C	1,000 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)	
		Skin			
		STEL	250 ppm 325 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)	
		Skin			

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis	
Aniline	62-53-3	Aniline	0.5 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)	
Remarks		End of shift (As soon as possible after exposure ceases)				

Methanol	67-56-1	Methanol	15 mg/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). Tightly fitting safety goggles

Skin protection

required

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter type ABEK

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.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- a) Appearance Form: clear, liquid
Color: yellow
- 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 310 °C 590 °F - lit.

g)	Flash point	110 °C (230 °F) - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapor pressure	No data available
l)	Vapor density	No data available
m)	Density	1.07 g/mL 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	Not classified as explosive.
t)	Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 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.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Exposure to moisture. Exposure to sunlight.

Strong heating.

10.5 Incompatible materials

Strong oxidizing agents, Water

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: Mixture causes burns.

Remarks: No data available

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye damage.

Risk of blindness!

Respiratory or skin sensitization

Mixture may cause an allergic skin reaction.

Germ cell mutagenicity

Evidence of genetic defects.

Carcinogenicity

Evidence of a carcinogenic effect.

IARC: 2A - Group 2A: Probably carcinogenic to humans (Aniline)

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

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Mixture causes damage to organs through prolonged or repeated exposure.

- Blood

Aspiration hazard

No data available

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Inhalation of vapors may cause:, Cough, Headache, Nausea, Skin contact may provoke the following symptoms:, allergic dermatitis

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Components

N-[3-(Trimethoxysilyl)propyl]aniline

Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: 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

Reproductive toxicity

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

Aniline

Acute toxicity

LD50 Oral - Rat - 250 mg/kg

Remarks: (RTECS)

LC50 Inhalation - Rat - 4 h - 3.3 mg/l - vapor

Remarks: (Lit.)

(Regulation (EC) No 1272/2008, Annex VI)

LC50 Inhalation - Rat - 4 h - 3.3 mg/l - vapor

Remarks: (Lit.)

(Regulation (EC) No 1272/2008, Annex VI)

LD50 Dermal - Rabbit - 840 mg/kg

Remarks: (Lit.)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

Remarks: (Lit.)

Serious eye damage/eye irritation

Remarks: Causes serious eye damage.

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

Respiratory or skin sensitization

May cause allergic skin reaction. Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Germ cell mutagenicity

Suspected of causing genetic defects.

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Result: positive

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster lung cells

Result: positive

Test Type: unscheduled DNA synthesis assay

Test system: rat hepatocytes

Result: negative

Remarks: (ECHA)

Method: OECD Test Guideline 474

Species: Rat - male - Bone marrow

Result: positive

Method: OECD Test Guideline 475

Species: Mouse - male and female - Bone marrow

Result: positive

Method: OECD Test Guideline 475

Species: Rat - male - Bone marrow

Result: positive

Method: OECD Test Guideline 478

Species: Rat - male

Result: negative

Carcinogenicity

Suspected of causing cancer.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Causes damage to organs through prolonged or repeated exposure.

- Blood

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

Aspiration hazard

No data available

Methanol

Acute toxicity

Acute toxicity estimate Oral - 100.1 mg/kg

(Expert judgment)

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

Symptoms: Nausea, Vomiting

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l - vapor

(Expert judgment)

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

Symptoms: Irritation symptoms in the respiratory tract.

Acute toxicity estimate Dermal - 300.1 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: No skin irritation

Remarks: (ECHA)

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

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

Remarks: (ECHA)

Respiratory or skin sensitization

Sensitisation test: - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Based on available data the classification criteria are not met.

Test Type: Ames test

Test system: *Salmonella typhimurium*

Result: negative

Test Type: *In vitro* mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female - Bone marrow

Result: negative

Carcinogenicity

Did not show carcinogenic effects in animal experiments.

Reproductive toxicity

Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

Causes damage to organs. - Eyes, Central nervous system

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

Acute oral toxicity - Nausea, Vomiting

Acute inhalation toxicity - Irritation symptoms in the respiratory tract.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

SECTION 12: Ecological information

12.1 Toxicity

Mixture

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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Components

N-[3-(Trimethoxysilyl)propyl]aniline

No data available

Aniline

Toxicity to fish

flow-through test LC50 - *Oncorhynchus mykiss* (rainbow trout)

- 10.6 mg/l - 96.0 h

Remarks: (ECHA)

Toxicity to daphnia
and other aquatic
invertebrates

semi-static test EC50 - *Daphnia magna* (Water flea) - 0.16 mg/l

- 48 h

(US-EPA)

Toxicity to algae	static test ErC50 - Chlorella pyrenoidosa - 175 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	EC50 - activated sludge - 2,500 mg/l - 10 min Remarks: (Lit.)
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Pimephales promelas (fathead minnow) - 0.39 mg/l - 32 d Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	flow-through test NOEC - Daphnia magna (Water flea) - 0.01 mg/l - 21 d (US-EPA)

Methanol

Toxicity to fish	flow-through test LC50 - Lepomis macrochirus (Bluegill) - 15,400.0 mg/l - 96 h (US-EPA)
Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - Daphnia magna (Water flea) - 18,260 mg/l - 96 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - ca. 22,000.0 mg/l - 96 h (OECD Test Guideline 201)
Toxicity to bacteria	static test IC50 - activated sludge - > 1,000 mg/l - 3 h (OECD Test Guideline 209)
Toxicity to fish(Chronic toxicity)	NOEC - Oryzias latipes (Orange-red killifish) - 7,900 mg/l - 200 h Remarks: (External MSDS)

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: 3267 Class: 8 Packing group: II
Proper shipping name: Corrosive liquid, basic, organic, n.o.s. (N-[3-(Trimethoxysilyl)propyl]aniline) (N-[3-(Trimethoxysilyl)propyl]aniline)
Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG

UN number: 3267 Class: 8 Packing group: II EMS-No: F-A, S-B
Proper shipping name: CORROSIVE LIQUID, BASIC, ORGANIC, N.O.S. (N-[3-(Trimethoxysilyl)propyl]aniline) (N-[3-(Trimethoxysilyl)propyl]aniline)

IATA

UN number: 3267 Class: 8 Packing group: II
Proper shipping name: Corrosive liquid, basic, organic, n.o.s. (N-[3-(Trimethoxysilyl)propyl]aniline) (N-[3-(Trimethoxysilyl)propyl]aniline)

SECTION 15: Regulatory information

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Aniline	62-53-3	5000	

SARA 304 Extremely Hazardous Substances Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Aniline	62-53-3	5000	

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

Components	CAS-No.	Component TPQ (lbs)
Aniline	62-53-3	1000

SARA 313

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

Aniline 62-53-3 $\geq 1\% < 5\%$

US State Regulations

Massachusetts Right To Know

Aniline 62-53-3

Pennsylvania Right To Know

Aniline 62-53-3
Methanol 67-56-1

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Aniline

62-53-3

Washington Chemicals of High Concern

Aniline

62-53-3

California Prop. 65

WARNING: This product can expose you to chemicals including Aniline, which is/are known to the State of California to cause cancer, and Methanol, which is/are known to the State of California to cause birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov.

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

... All substances listed as active on the 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.

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**Millipore
Sigma**