

SAFETY DATA SHEET

Version 6.3
Revision Date 08/18/2021
Print Date 06/01/2022

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

Product name : Aniline- $^{13}\text{C}_6$

Product Number : 485497
Brand : Aldrich
CAS-No. : 100849-37-4

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 4), H227
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
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 1), H400
Long-term (chronic) aquatic hazard (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)

H227	Combustible liquid.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H341	Suspected of causing genetic defects.
H351	Suspected of causing cancer.
H372	Causes damage to organs (Blood) through prolonged or repeated exposure.
H410	Very toxic to aquatic life with long lasting effects.

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.
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.
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 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P302 + P352 + P312	IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.
P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. 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.
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.
P391	Collect spillage.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
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 - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula : $^{13}\text{C}_6\text{H}_7\text{N}$
Molecular weight : 99.03 g/mol
CAS-No. : 100849-37-4

Component	Classification	Concentration
Aniline-13C6		
	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: 10 M-Factor - Aquatic Chronic: 1	<= 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

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

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

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

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

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)

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

Remove container from danger zone and cool with water. 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. 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.

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

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

Storage stability

Recommended storage temperature

2 - 8 °C

Storage class

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

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-13C6	100849-37-4	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		

		TWA	2 ppm 8 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Aniline-13C6	100849-37-4	Aniline		Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			
		Aniline		Released from hemoglobin in blood	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			
		p-Aminophenol	50 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

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: liquid

b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: -6 °C (21 °F) - lit.
f) Initial boiling point and boiling range	184 °C 363 °F - lit.
g) Flash point	70 °C (158 °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	1.087 g/mL at 25 °C (77 °F)1.087 g/cm ³ at 25 °C (77 °F)
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	No data available

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) .
May discolor on exposure to light.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Strong 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

LD50 Oral - Rat - 250 mg/kg

Remarks: (RTECS)

The value is given in analogy to the following substances: Aniline

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

Remarks: (Lit.)

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

The value is given in analogy to the following substances: Aniline

LD50 Dermal - Rabbit - 840 mg/kg

Remarks: (Lit.)

The value is given in analogy to the following substances: Aniline

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

Remarks: (Lit.)

The value is given in analogy to the following substances: Aniline

Serious eye damage/eye irritation

Causes serious eye damage. Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2) The value is given in analogy to the following substances:

Respiratory or skin sensitization

May cause allergic skin reaction. Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2) The value is given in analogy to the following substances:

Germ cell mutagenicity

Suspected of causing genetic defects.

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: The value is given in analogy to the following substances: Aniline Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: positive

Remarks: The value is given in analogy to the following substances: Aniline Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: positive

Remarks: The value is given in analogy to the following substances: Aniline
Test Type: unscheduled DNA synthesis assay

Test system: rat hepatocytes

Metabolic activation: without metabolic activation

Result: negative

Remarks: (ECHA)

The value is given in analogy to the following substances: Aniline

Test Type: Micronucleus test

Species: Rat

Cell type: Bone marrow

Application Route: Oral

Method: OECD Test Guideline 474

Result: positive

Remarks: The value is given in analogy to the following substances: Aniline

Test Type: Micronucleus test

Species: Mouse

Cell type: Bone marrow

Application Route: Intraperitoneal

Method: OECD Test Guideline 475

Result: positive

Remarks: The value is given in analogy to the following substances: Aniline

Test Type: Chromosome aberration test

Species: Rat

Cell type: Bone marrow

Application Route: Oral

Method: OECD Test Guideline 475

Result: positive

Remarks: The value is given in analogy to the following substances: Aniline

Test Type: dominant lethal test

Species: Rat

Application Route: Intraperitoneal

Method: OECD Test Guideline 478

Result: negative

Remarks: The value is given in analogy to the following substances: Aniline

Carcinogenicity

Suspected of causing cancer.

IARC: 2A - Group 2A: Probably carcinogenic to humans (Aniline-13C6)

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

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)

The value is given in analogy to the following substances: Aniline

Aspiration hazard

No data available

11.2 Additional Information

Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. Onset may be delayed 2 to 4 hours or longer., Cyanosis, Headache, Vomiting, Nausea, Incoordination., fatigue, Dizziness, Drowsiness, Confusion., Weakness, Unconsciousness, Symptoms may be delayed.
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish	flow-through test LC50 - Oncorhynchus mykiss (rainbow trout) - 10.6 mg/l - 96.0 h Remarks: (ECHA) The value is given in analogy to the following substances: Aniline
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Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - Daphnia magna (Water flea) - 0.16 mg/l - 48 h (US-EPA) Remarks: The value is given in analogy to the following substances: Aniline
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Toxicity to algae	static test ErC50 - Chlorella pyrenoidosa - 175 mg/l - 72 h (OECD Test Guideline 201) Remarks: The value is given in analogy to the following substances: Aniline
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Toxicity to bacteria	EC50 - activated sludge - 2,500 mg/l - 10 min Remarks: (Lit.) The value is given in analogy to the following substances: Aniline
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12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 30 d Result: ca.90 % - Readily biodegradable. (OECD Test Guideline 301D) Remarks: The value is given in analogy to the following substances: Aniline
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12.3 Bioaccumulative potential

Bioaccumulation Danio rerio (zebra fish) - < 0.1 mg/l(Aniline-13C6)

Bioconcentration factor (BCF): 2.6

Remarks: The value is given in analogy to the following substances:
Aniline

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: 1547 Class: 6.1

Packing group: II

Proper shipping name: Aniline

Reportable Quantity (RQ): 5000 lbs

1) Marine pollutant: yes Poison Inhalation Hazard: No

IMDG

UN number: 1547 Class: 6.1

Packing group: II

EMS-No: F-A, S-A

Proper shipping name: ANILINE

Marine pollutant : yes

Marine pollutant : yes

IATA

UN number: 1547 Class: 6.1

Packing group: II

Proper shipping name: Aniline

SECTION 15: Regulatory information

SARA 302 Components

Aniline-13C6

CAS-No.

100849-37-4

Revision Date

2007-03-01

SARA 313 Components

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

	CAS-No.	Revision Date
Aniline-13C6	100849-37-4	2007-03-01

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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