

3-[3-(Trifluoromethyl)-3H-diaziren-3-yl]aniline

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
 SDS ID: 3640300
 Issue date: 2/13/2018 Revision date: 8/20/2024 Version: 1.1

SECTION 1: Identification

1.1. Identification

Product form : Substance
 Substance name : 3-[3-(Trifluoromethyl)-3H-diaziren-3-yl]aniline
 CAS-No. : 130973-96-5
 Product code : 3640-3-00
 Formula : C₈H₆F₃N₃
 Other means of identification : MFCD24646280

1.2. Recommended use and restrictions on use

Use of the substance/mixture : Laboratory chemicals
 Manufacture of substances
 Scientific research and development

1.3. Supplier

SynQuest Laboratories, Inc.
 P.O. Box 309
 Alachua, FL, Alachua, 32615
 United States of America
 T (386) 462-0788 - F (386) 462-7097
info@synquestlabs.com - www.synquestlabs.com

1.4. Emergency telephone number

Emergency number : (844) 523-4086 (3E Company - Account 10069)

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS US classification

Acute toxicity (oral) Category 4	H302	Harmful if swallowed
Acute toxicity (dermal) Category 4	H312	Harmful in contact with skin
Acute toxicity (inhalation) Category 4	H332	Harmful if inhaled
Skin corrosion/irritation Category 2	H315	Causes skin irritation
Serious eye damage/eye irritation Category 2A	H319	Causes serious eye irritation
Specific target organ toxicity – Single exposure, Category 3, Respiratory tract irritation	H335	May cause respiratory irritation

Full text of H statements : see section 16

2.2. GHS Label elements, including precautionary statements

GHS US labeling

Hazard pictograms (GHS US) :



Signal word (GHS US) : Warning
 Hazard statements (GHS US) : H302+H312+H332 - Harmful if swallowed, in contact with skin or if inhaled
 H315 - Causes skin irritation

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Precautionary statements (GHS US)

- H319 - Causes serious eye irritation
- H335 - May cause respiratory irritation
- P261 - Avoid breathing fumes, mist, spray, vapors.
- 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.
- P280 - Wear protective gloves/protective clothing/eye protection/face protection.
- P301+P312 - If swallowed: Call a POISON CENTER or doctor/ physician if you feel unwell
- P302+P352 - If on skin: Wash with plenty of soap and water
- P304+P340 - If inhaled: Remove person to fresh air and keep 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.
- P312 - Call a POISON CENTER or doctor/physician if you feel unwell
- P321 - Specific treatment (see supplemental first aid instructions on this label)
- P322 - Specific treatment (see supplemental first aid instruction on this label)
- P330 - Rinse mouth.
- P332+P313 - If skin irritation occurs: Get medical advice/attention.
- P337+P313 - If eye irritation persists: Get medical advice/attention.
- P362+P364 - Take off contaminated clothing and wash it before reuse.
- 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. Other hazards which do not result in classification

No additional information available

2.4. Unknown acute toxicity (GHS US)

No additional information available

SECTION 3: Composition/Information on ingredients

3.1. Substances

Substance type : Mono-constituent

Name	Product identifier	%	GHS US classification
3-[3-(Trifluoromethyl)-3H-diaziren-3-yl]aniline (Main constituent)	CAS-No.: 130973-96-5	≤ 100	Acute Tox. 4 (Oral), H302 Acute Tox. 4 (Dermal), H312 Acute Tox. 4 (Inhalation), H332 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335

Full text of hazard classes and H-statements : see section 16

3.2. Mixtures

Not applicable

SECTION 4: First-aid measures

4.1. Description of first aid measures

First-aid measures general : In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Move the affected personnel away from the contaminated area.

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First-aid measures after inhalation	: Remove person to fresh air and keep comfortable for breathing. If not breathing, give artificial respiration. Get immediate medical advice/attention.
First-aid measures after skin contact	: Wash with plenty of soap and water. Get immediate medical advice/attention.
First-aid measures after eye contact	: Remove contact lenses, if present and easy to do. Continue rinsing. Immediately flush eyes thoroughly with water for at least 15 minutes. Get immediate medical advice/attention.
First-aid measures after ingestion	: Due to its physical form, exposure to this chemical is not likely. Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get immediate medical advice/attention.

4.2. Most important symptoms and effects (acute and delayed)

Symptoms/effects	: The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.
Symptoms/effects after inhalation	: May cause drowsiness or dizziness.

4.3. Immediate medical attention and special treatment, if necessary

No additional information available

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media	: Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media appropriate for surrounding fire.
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5.2. Specific hazards arising from the chemical

Fire hazard	: Thermal decomposition generates: Carbon oxides. Hydrogen fluoride. Nitrogen oxides.
Explosion hazard	: Risk of explosion if heated under confinement. Use water spray or fog for cooling exposed containers.

5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions	: In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.
Protection during firefighting	: Wear gas tight chemically protective clothing in combination with self contained breathing apparatus. For further information refer to section 8: "Exposure controls/personal protection".

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures	: Evacuate unnecessary personnel. Ensure adequate air ventilation. Do not breathe gas, fumes, vapor or spray.
6.1.1. For non-emergency personnel	
Emergency procedures	: Only qualified personnel equipped with suitable protective equipment may intervene.
6.1.2. For emergency responders	
Protective equipment	: Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".
Emergency procedures	: Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level.

6.2. Environmental precautions

Avoid release to the environment. Notify authorities if product enters sewers or public waters.

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6.3. Methods and material for containment and cleaning up

For containment	: Stop leak if safe to do so. Dike for recovery or absorb with appropriate material.
Methods for cleaning up	: Take up large spills with pump or vacuum and finish with dry chemical absorbent. Use explosion-proof equipment. Take up small spills with dry chemical absorbent. Sweep or shovel spills into appropriate container for disposal. Ventilate area.
Other information	: For disposal of solid materials or residues refer to section 13 : "Disposal considerations".

6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling	: Do not handle until all safety precautions have been read and understood. Ensure good ventilation of the work station. Do not breathe fumes, mist, spray, vapors. Wear personal protective equipment. Avoid contact with skin and eyes.
Hygiene measures	: Handle in accordance with good industrial hygiene and safety procedures. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures	: Comply with applicable regulations.
Storage conditions	: Keep container closed when not in use.
Incompatible materials	: Refer to Section 10 on Incompatible Materials.
Storage area	: Store in dry, cool, well-ventilated area. Light sensitive.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Appropriate engineering controls

Appropriate engineering controls	: Ensure good ventilation of the work station. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.
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8.3. Individual protection measures/Personal protective equipment

Hand protection:
protective gloves. 29 CFR 1910.138: Hand Protection
Eye protection:
Chemical goggles or safety glasses. Face shield. 29 CFR 1910.133: Eye and Face Protection
Skin and body protection:
Wear suitable protective clothing
Respiratory protection:
In case of inadequate ventilation wear respiratory protection. 29 CFR 1910.134: Respiratory Protection

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Personal protective equipment symbol(s):



Other information:

Safety shoes. 29 CFR 1910.136: Foot Protection.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Color	: No data available
Odor	: No data available
Odor threshold	: No data available
pH	: No data available
Melting point	: No data available
Freezing point	: No data available
Boiling point	: 68 – 70 °C
Flash point	: No data available
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: No data available
Vapor pressure	: No data available
Relative vapor density at 20 °C	: No data available
Relative density	: No data available
Molecular mass	: 201.1485 g/mol
Solubility	: No data available
Partition coefficient n-octanol/water (Log Pow)	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosion limits	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

The product is stable at normal handling and storage conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Keep away from heat, sparks and flame.

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10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced. Hazardous decomposition products in case of fire, see Section 5.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity (oral) : Harmful if swallowed.
Acute toxicity (dermal) : Harmful in contact with skin.
Acute toxicity (inhalation) : Harmful if inhaled.

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ATE US (oral)	500 mg/kg body weight
ATE US (dermal)	1100 mg/kg body weight
ATE US (gases)	4500 ppmV/4h
ATE US (vapors)	11 mg/l/4h
ATE US (dust, mist)	1.5 mg/l/4h

Skin corrosion/irritation : Causes skin irritation.
Serious eye damage/irritation : Causes serious eye irritation.
Respiratory or skin sensitization : Not classified
Germ cell mutagenicity : Not classified
Carcinogenicity : Not classified
Reproductive toxicity : Not classified
STOT-single exposure : May cause respiratory irritation.
STOT-repeated exposure : Not classified
Aspiration hazard : Not classified
Viscosity, kinematic : No data available
Symptoms/effects : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.
Symptoms/effects after inhalation : May cause drowsiness or dizziness.

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

12.2. Persistence and degradability

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Persistence and degradability	Rapidly degradable
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12.3. Bioaccumulative potential

No additional information available

12.4. Mobility in soil

No additional information available

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12.5. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Disposal methods

Waste treatment methods	: Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.
Product/Packaging disposal recommendations	: Dispose of contents/container in accordance with licensed collector's sorting instructions.
Additional information	: Recycle the material as far as possible.

SECTION 14: Transport information

14.1. UN number

Not regulated for transport

14.2. UN proper shipping name

Proper Shipping Name (DOT)	: Not applicable
Proper Shipping Name (TDG)	: Not applicable
Proper Shipping Name (IMDG)	: Not applicable
Proper Shipping Name (IATA)	: Not applicable

14.3. Transport hazard class(es)

DOT
Transport hazard class(es) (DOT) : Not applicable

TDG
Transport hazard class(es) (TDG) : Not applicable

IMDG
Transport hazard class(es) (IMDG) : Not applicable

IATA
Transport hazard class(es) (IATA) : Not applicable

14.4. Packing group

Packing group (DOT)	: Not applicable
Packing group (TDG)	: Not applicable
Packing group (IMDG)	: Not applicable
Packing group (IATA)	: Not applicable

14.5. Environmental hazards

Other information : No supplementary information available.

14.6. Special precautions for user

DOT
No data available

TDG
No data available

IMDG
No data available

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IATA
No data available

14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

SECTION 15: Regulatory information

15.1. US Federal regulations

All components of this product are present and listed as Active on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory, except for:		
3-[3-(Trifluoromethyl)-3H-diaziren-3-yl]aniline	CAS-No. 130973-96-5	100%

15.2. International regulations

CANADA
No additional information available

EU-Regulations
No additional information available

National regulations
No additional information available

15.3. US State regulations

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

SECTION 16: Other information

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Revision date : 8/20/2024

Full text of H-phrases	
H302	Harmful if swallowed
H312	Harmful in contact with skin
H315	Causes skin irritation
H319	Causes serious eye irritation
H332	Harmful if inhaled
H335	May cause respiratory irritation

NFPA health hazard

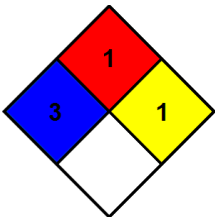
NFPA fire hazard

NFPA reactivity

: 3 - Materials that, under emergency conditions, can cause serious or permanent injury.

: 1 - Materials that must be preheated before ignition can occur.

: 1 - Materials that in themselves are normally stable but can become unstable at elevated temperatures and pressures.



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Hazard Rating

- Health : 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given
- Flammability : 1 Slight Hazard - Materials that must be preheated before ignition will occur. Includes liquids, solids and semi solids having a flash point above 200 F. (Class IIIB)
- Physical : 1 Slight Hazard - Materials that are normally stable but can become unstable (self-react) at high temperatures and pressures. Materials may react non-violently with water or undergo hazardous polymerization in the absence of inhibitors.

Safety Data Sheet (SDS), USA

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 offered solely for your consideration, investigation, and verification. It does not represent any guarantee of the properties of the product nor that the hazard precautions or procedures described are the only ones which exist. SynQuest shall not be held liable or any damage resulting from handling or from contact with the above product.