

SAFETY DATA SHEET

according to 1907/2006/EC, Article 3

Version no. : 2.0
Prepared on : 02.04.2026
Revised on : -

SECTION 1: Identification of the substance/mixture and of the company/undertaking.

1.1 Product identifiers

Product name 3-(Trifluoromethyl)aniline
Product Number PSR50419
Brand PureSynth research chemicals
CAS No. 98-16-8

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

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company PureSynth Research Chemicals GmbH
64683 Einhausen Marie-Curie-StraBe. 3, Germany

1.4 Emergency telephone number

Worldwide Helpline No.: 1800-8908-260

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Acute toxicity, Category 4	H302: Harmful if swallowed.
Acute toxicity, Category 4	H312: Harmful in contact with skin.
Skin irritation, Category 2	H315: Causes skin irritation.
Serious eye damage, Category 1	H318: Causes serious eye damage.
Long-term (chronic) aquatic hazard, Category 2	H411: Toxic to aquatic life with long lasting effects.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram



Signal word

Danger

Hazard statement(s)

H302 + H312	Harmful if swallowed or in contact with skin.
H315	Causes skin irritation.
H318	Causes serious eye irritation.
H411	Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P264	Wash skin thoroughly after handling.
P273	Avoid release to the environment.

P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.
P302 + P352 + P312	IF ON SKIN: Wash with plenty of water. 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.
Supplemental Hazard Statements	none

2.3 Other hazards:

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher

SECTION 3: Composition / information on ingredients

3.1 Substances

Common names & Synonyms	Mol. formula	CAS number
3-aminobenzotrifluoride	C ₇ H ₆ F ₃ N	98-16-8
Component	Classification	Concentration
3-(Trifluoromethyl)aniline	Acute toxicity estimate Acute dermal toxicity: 1100.1 mg/kg	>= 90 - <= 100

SECTION 4: First aid measures

Description of first aid measures

General advice	Show this 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. Immediately call in ophthalmologist. Remove contact lenses.
If swallowed	After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.
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
Indication of any immediate medical attention and special treatment needed	No data available

SECTION 5: Firefighting measures

Extinguishing media	
Suitable extinguishing media	Water Foam Carbon dioxide (CO ₂)

Unsuitable extinguishing media	Dry powder
Special hazards arising from the substance or mixture	For this substance/mixture no limitations of extinguishing agents are given. Combustible. Vapours 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. Carbon oxides Nitrogen oxides (NOx) Hydrogen fluoride
Advice for fire-fighters	Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.
Further information	Remove container from danger zone and cool with water. Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures	Advice for non-emergency personnel: Do not breathe vapours, 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.
Environmental precautions	Do not let product enter drains.
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. Dispose of properly. Clean up affected area. Avoid generation of dusts.
Reference to other sections	For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling	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.
Conditions for safe storage, including any incompatibilities	Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons. Storage class (TRGS 510): 6.1A, Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials
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

Control parameters	Ingredients with workplace control parameters
Exposure controls	
Appropriate engineering controls	No data available
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

Hand protection

Material: natural latex
Break through time: 10 min
Glove thickness: 0.6 mm
Protective index: Splash contact

Material: butyl-rubber
Break through time: 480 min
Glove thickness: 0.7 mm
Protective index: Full contact

Skin and Body Protection

Respiratory protection

Remarks: 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 protective clothing 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.
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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

Appearance	Form: Liquid Colour: Colourless
Odour	No data available
pH - Value	No data available
Density	1.29 g/cm ³ (25 °C) Method: lit.
Boiling Point	187 °C Method: lit.
Melting Point	5 - 6 °C Method: lit.
Solubility in water	4.68 g/l (20 °C) pH: 5 Method: Regulation (EC) No. 440/2008, Annex, A.6 GLP: yes soluble
Flash point	87 °C Method: closed cup
Vapour pressure	No data available
Auto-ignition temperature	No data available
Vapour density	No data available
Flammability (solid, gas)	No data available
Evaporation rate	No data available
Partition coefficient: n- octanol / water	log Pow: 2.09 (30 °C) pH: 5.9 Method: Regulation (EC) No. 440/2008, Annex, A.8 GLP: yes Bioaccumulation is not expected.
Viscosity	No data available
Explosive properties	Not classified as explosive.
Upper / lower flammability or explosive limits	No data available
Oxidizing properties	No data available

Other safety information: No data available

SECTION 10: Stability and reactivity

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.
Chemical stability	The product is chemically stable under standard ambient conditions (room temperature).
Possibility of hazardous reactions	No data available
Condition to avoid	Strong heating.
Incompatible materials	Strong oxidizing agents
Hazardous decomposition products	In the event of fire: see section 5

SECTION 11: Toxicological information

Acute toxicity	LD50 Oral - Rat - 477 mg/kg Remarks: Behavioral: Somnolence (general depressed activity). (RTECS) Inhalation: No data available Acute toxicity estimate Dermal - 1100.1 mg/kg
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	(Expert judgement)
	LD50 Dermal - Rabbit - 1330 mg/kg
	Remarks: Behavioral: Somnolence (general depressed activity).
	Lungs, Thorax, or Respiration: Dyspnea.
	Prolonged skin contact may cause skin irritation and/or dermatitis.
	(RTECS)
Skin corrosion/irritation	Skin - In vitro study
	Result: irritating
	Remarks: (ECHA)
	Skin - In vitro study
	Result: non-corrosive
Serious eye damage/eye irritation	Eyes - Rabbit
	Result: Irreversible effects on the eye
	Remarks: (ECHA)
Respiratory or skin sensitization	Local lymph node assay (LLNA) - Mouse
	Result: Not a skin sensitizer.
	(OECD Test Guideline 429)
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
Additional Information	The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.
	Cough, Shortness of breath, Headache, Nausea, Vomiting, May cause cyanosis., prolonged or repeated exposure can cause: Dizziness, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

Toxicity

Toxicity to fish	No data available
Toxicity to daphnia and other aquatic invertebrates	EC50 (Daphnia magna (Water flea)): 2.7 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Remarks: (ECOTOX Database)
Toxicity to algae	No data available
Toxicity to bacteria	No data available
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	No data available
Persistence and degradability	Test Type: aerobic Inoculum: activated sludge, non-adapted Concentration: 10 mg/l

	Result: Not readily biodegradable.
	Biodegradation: 4 %
	Exposure time: 28 d
	Method: OECD Test Guideline 301B
	GLP: yes
Bioaccumulation	log Pow: 2.09 (30 °C)
	pH: 5.9 Method: Regulation (EC) No. 440/2008, Annex, A.8
	GLP: yes
	Remarks: Bioaccumulation is not expected.
Mobility in soil	No data available
Results of PBT and vPvB assessment	This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.
Endocrine disrupting properties	The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.
Other adverse effects	Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Waste treatment methods	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.
Contaminated packaging	No data available.

SECTION 14: Transport information

	UN no.	UN proper shipping name	Hazard Class(es)	Packaging group	Marine Pollutant
ADR / RID	2948	3-TRIFLUOROMETHYLANILINE	6.1	II	no
IMDG	2948	3-TRIFLUOROMETHYLANILINE	6.1	II	no
IATA	2948	3-Trifluoromethylaniline	6.1	II	-

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII)	Conditions of restriction for the following entries should be considered: Number on list 3
REACH - Candidate List of Substances of Very High Concern for Authorisation (Article 59).	Not applicable
Regulation (EU) No 2024/590 on substances that deplete the ozone layer	Not applicable
Regulation (EU) 2019/1021 on persistent organic pollutants (recast)	Not applicable
REACH - List of substances subject to authorisation (Annex XIV)	Not applicable
Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.	E2 ENVIRONMENTAL HAZARDS

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

The information in this SDS 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. The user must be determined suitability of this information for his application.