

SAFETY DATA SHEET

Version 5.2
Revision Date 06/27/2014
Print Date 11/15/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : 4-(Trifluoromethyl)phenyl isothiocyanate

Product Number : 476099

Brand : Aldrich

CAS-No. : 1645-65-4

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 : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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

Respiratory sensitisation (Category 1), H334

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)

H314

Causes severe skin burns and eye damage.

H334

May cause allergy or asthma symptoms or breathing difficulties if inhaled.

Precautionary statement(s)

P260

Do not breathe dust or mist.

P264

Wash skin thoroughly after handling.

P280

Wear protective gloves/ protective clothing/ eye protection/ face protection.

P285

In case of inadequate ventilation wear respiratory protection.

P301 + P330 + P331

IF SWALLOWED: rinse mouth. Do NOT induce vomiting.

P303 + P361 + P353

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

P304 + P340

IF INHALED: Remove victim to fresh air and keep at rest in a position

P305 + P351 + P338	comfortable for breathing. IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310	Immediately call a POISON CENTER or doctor/ physician.
P321	Specific treatment (see supplemental first aid instructions on this label).
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

Lachrymator.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula	: C ₈ H ₄ F ₃ NS
Molecular Weight	: 203.18 g/mol
CAS-No.	: 1645-65-4

Hazardous components

Component	Classification	Concentration
4-(Trifluoromethyl)phenyl isothiocyanate		
	Skin Corr. 1B; Eye Dam. 1; Resp. Sens. 1; H314, H334	-

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides, nitrogen oxides (NO_x), Sulphur oxides, Hydrogen fluoride

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information
no data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.
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

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.
Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Store under inert gas. Moisture sensitive.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance	Form: solid Colour: tan
b) Odour	no data available
c) Odour Threshold	no data available
d) pH	no data available
e) Melting point/freezing point	Melting point/range: 39 - 43 °C (102 - 109 °F) - lit.
f) Initial boiling point and boiling range	81 °C (178 °F) at 15 hPa (11 mmHg) - lit.
g) Flash point	113 °C (235 °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) Vapour pressure	no data available
l) Vapour density	no data available
m) Relative density	no data available
n) Water solubility	no data available
o) Partition coefficient: n-octanol/water	no data available
p) Auto-ignition 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

10. STABILITY AND REACTIVITY

10.1 Reactivity

no data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

Heat. Avoid moisture.

10.5 Incompatible materials

Alcohols, Strong bases, Amines, acids, Strong oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - no data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

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 sensitisation

Germ cell mutagenicity

no data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

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

Additional Information

RTECS: Not available

Cough, Shortness of breath, Headache, Nausea, Vomiting

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

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 3261 Class: 8 Packing group: II
Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (4-(Trifluoromethyl)phenyl isothiocyanate)
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG

UN number: 3261 Class: 8 Packing group: II EMS-No: F-A, S-B
Proper shipping name: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (4-(Trifluoromethyl)phenyl isothiocyanate)
Marine pollutant: No

IATA

UN number: 3261 Class: 8 Packing group: II
Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (4-(Trifluoromethyl)phenyl isothiocyanate)

15. REGULATORY INFORMATION

SARA 302 Components

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

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

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
4-(Trifluoromethyl)phenyl isothiocyanate	1645-65-4	

New Jersey Right To Know Components

	CAS-No.	Revision Date
4-(Trifluoromethyl)phenyl isothiocyanate	1645-65-4	

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Eye Dam.	Serious eye damage
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
Resp. Sens.	Respiratory sensitisation
Skin Corr.	Skin corrosion

HMIS Rating

Health hazard:	3
Chronic Health Hazard:	*
Flammability:	1
Physical Hazard	0

NFPA Rating

Health hazard:	3
Fire Hazard:	1
Reactivity Hazard:	0

Further information

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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.

Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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