

# Safety data sheet

according to 1907/2006/EC, Article 31

Revision: 18.01.2010

Printing date 02.07.2013

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

Trade name

**2-Nitro-4-(trifluoromethyl)benzonitrile**

Stock number:

L10557

CAS Number:

778-94-9

EC number:

212-298-1

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

Identified use:

SU24 Scientific research and development

**1.3 Details of the supplier of the safety data sheet**

Manufacturer/Supplier:

Alfa Aesar GmbH & Co.KG  
A Johnson Matthey Company  
Zeppelinstr. 7b  
76185 Karlsruhe / Germany  
Tel: +49 (0) 721 84007 280  
Fax: +49 (0) 721 84007 300  
Email: tech@alfa.com  
www.alfa.com

Informing department:

Product safety Tel + +049 (0) 7275 988687-0

**1.4 Emergency telephone number:**

Carechem 24: +44 (0) 1235 239 670 (Multi-language emergency number)

Poison Information Center Mainz

www.giftinfo.uni-mainz.de Telephone: +49(0)6131/19240

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture**

Classification according to Regulation (EC) No 1272/2008



GHS06 skull and crossbones

Acute Tox. 3 H311 Toxic in contact with skin.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Acute Tox. 4 H332 Harmful if inhaled.

Skin Irrit. 2 H315 Causes skin irritation.

Eye Irrit. 2 H319 Causes serious eye irritation.

**Classification according to Directive 67/548/EEC or Directive 1999/45/EC**

Xn; Harmful

R20/21/22: Harmful by inhalation, in contact with skin and if swallowed.

Xi; Irritant

R36/38: Irritating to eyes and skin.

**Information concerning particular hazards for human and environment:**

Other hazards that do not result in classification

Not applicable

No information known.

**2.2 Label elements**

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms

Signal word

Hazard statements

The substance is classified and labelled according to the CLP regulation.

GHS06

Danger

H302 Harmful if swallowed.

H311 Toxic in contact with skin.

H332 Harmful if inhaled.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

P280

Wear protective gloves / protective clothing.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if

present and easy to do. Continue rinsing.

P309

IF exposed or if you feel unwell:

P310 Immediately call a POISON CENTER or doctor/physician.

**2.3 Other hazards**

Results of PBT and vPvB assessment

PBT:

Not applicable.

vPvB:

Not applicable.

**SECTION 3: Composition/information on ingredients****3.1 Substances**

CAS# Designation:

778-94-9 2-Nitro-4-(trifluoromethyl)benzonitrile

Identification number(s):

212-298-1

EC number:

212-298-1

**SECTION 4: First aid measures****4.1 Description of first aid measures**

After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

After skin contact

Seek immediate medical advice.

Instantly wash with water and soap and rinse thoroughly.

After eye contact

Seek immediate medical advice.

Rinse opened eye for several minutes under running water. Then consult doctor.

After swallowing

Seek medical treatment.

**4.2 Most important symptoms and effects, both acute and delayed**

No further relevant information available.

**4.3 Indication of any immediate medical attention and special treatment needed**

No further relevant information available.

**SECTION 5: Firefighting measures****5.1 Extinguishing media**

Suitable extinguishing agents

CO2, extinguishing powder or water jet. Fight larger fires with water jet or alcohol-resistant foam.

**5.2 Special hazards arising from the substance or mixture**

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

Nitrogen oxides (NOx)

Hydrogen fluoride (HF)

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## 5.3 Advice for firefighters

### Protective equipment:

Hydrogen cyanide (HCN)

Wear self-contained breathing apparatus.  
Wear full protective suit.

## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.  
Ensure adequate ventilation.

### 6.2 Environmental precautions:

Do not allow material to be released to the environment without proper governmental permits.  
Do not allow product to reach sewage system or water bodies.  
Do not allow to enter the ground/soil.

### 6.3 Methods and material for containment and cleaning up:

Dispose of contaminated material as waste according to item 13.  
Ensure adequate ventilation.

### Prevention of secondary hazards:

No special measures required.

### 6.4 Reference to other sections

See Section 7 for information on safe handling  
See section 8 for information on personal protection equipment.  
See Section 13 for information on disposal.

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Keep containers tightly sealed.  
Store in cool, dry place in tightly closed containers.  
Ensure good ventilation/exhaustion at the workplace.

### Information about protection against explosions and fires:

No information known.

### 7.2 Conditions for safe storage, including any incompatibilities

#### Storage Requirements to be met by storerooms and containers:

No special requirements.

#### Information about storage in one common storage facility:

Store away from oxidizing agents.

#### Further information about storage conditions:

Keep container tightly sealed.  
Store in cool, dry conditions in well sealed containers.  
No further relevant information available.

### 7.3 Specific end use(s)

## SECTION 8: Exposure controls/personal protection

### Additional information about design of technical systems:

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

### 8.1 Control parameters

#### Components with critical values that require monitoring at the workplace:

Not required.

#### Additional information:

No data

### 8.2 Exposure controls

#### Personal protective equipment

#### General protective and hygienic measures

The usual precautionary measures should be adhered to in handling the chemicals.

Keep away from foodstuffs, beverages and food.

Instantly remove any soiled and impregnated garments.

Wash hands during breaks and at the end of the work.

Avoid contact with the eyes and skin.

Maintain an ergonomically appropriate working environment.

Use breathing protection with high concentrations.

Check protective gloves prior to each use for their proper condition.

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

Impervious gloves

Not determined

Safety glasses

Face protection

Protective work clothing.

#### Breathing equipment:

#### Protection of hands:

#### Material of gloves

#### Penetration time of glove material

#### Eye protection:

#### Body protection:

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

#### General Information

##### Appearance:

Form: Crystalline powder

Colour: Yellow

Smell: Not determined

Odour threshold: Not determined.

pH-value: Not applicable.

#### Change in condition

Melting point/Melting range: 40-44 °C

Boiling point/Boiling range: 156-158 °C (18 mmHg)

Sublimation temperature / start: Not determined

Flash point: &gt; 110 °C

Inflammability (solid, gaseous): Not determined.

Ignition temperature: Not determined

Decomposition temperature: Not determined

Self-inflammability: Not determined.

Danger of explosion: Product is not explosive.

#### Critical values for explosion:

Lower: Not determined

Upper: Not determined

Steam pressure: Not applicable.

Density: Not determined

Relative density: Not determined.

Vapour density: Not applicable.

Evaporation rate: Not applicable.

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<b>Solubility in / Miscibility with</b>	
Water:	Insoluble
<b>Partition coefficient (n-octanol/water):</b>	Not determined.
<b>Viscosity:</b>	
dynamic:	Not applicable.
kinematic:	Not applicable.
<b>9.2 Other information</b>	No further relevant information available.

**SECTION 10: Stability and reactivity**

<b>10.1 Reactivity</b>	No information known.
<b>10.2 Chemical stability</b>	Stable under recommended storage conditions.
<b>Thermal decomposition / conditions to be avoided:</b>	No decomposition if used and stored according to specifications.
<b>10.3 Possibility of hazardous reactions</b>	No dangerous reactions known
<b>10.5 Incompatible materials:</b>	Oxidizing agents
<b>10.6 Hazardous decomposition products:</b>	Carbon monoxide and carbon dioxide Nitrogen oxides (NOx) Hydrogen fluoride Hydrogen cyanide (prussic acid)

**SECTION 11: Toxicological information**

<b>11.1 Information on toxicological effects</b>	
<b>Acute toxicity:</b>	Harmful if inhaled. Harmful in contact with skin. Harmful if swallowed. Danger by skin resorption.
<b>LD/LC50 values that are relevant for classification:</b>	No data
<b>Skin irritation or corrosion:</b>	Causes skin irritation.
<b>Eye irritation or corrosion:</b>	Causes serious eye irritation.
<b>Sensitization:</b>	No sensitizing effect known.
<b>Germ cell mutagenicity:</b>	No effects known.
<b>Carcinogenicity:</b>	No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.
<b>Reproductive toxicity:</b>	No effects known.
<b>Specific target organ system toxicity - repeated exposure:</b>	No effects known.
<b>Specific target organ system toxicity - single exposure:</b>	No effects known.
<b>Aspiration hazard:</b>	No effects known.
<b>Additional toxicological information:</b>	To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.



**SECTION 12: Ecological information**

<b>12.1 Toxicity</b>	
<b>Aquatic toxicity:</b>	No further relevant information available.
<b>12.2 Persistence and degradability</b>	No further relevant information available.
<b>12.3 Bioaccumulative potential</b>	No further relevant information available.
<b>12.4 Mobility in soil</b>	No further relevant information available.
<b>Additional ecological information:</b>	
<b>General notes:</b>	Do not allow material to be released to the environment without proper governmental permits. Water hazard class 1 (Self-assessment): slightly hazardous for water. Do not allow undiluted product or large quantities of it to reach ground water, water bodies or sewage system. Avoid transfer into the environment.
<b>12.5 Results of PBT and vPvB assessment</b>	
<b>PBT:</b>	Not applicable.
<b>vPvB:</b>	Not applicable.
<b>12.6 Other adverse effects</b>	No further relevant information available.

**SECTION 13: Disposal considerations**

<b>13.1 Waste treatment methods</b>	
<b>Recommendation</b>	Hand over to disposers of hazardous waste. Must be specially treated under adherence to official regulations. Consult state, local or national regulations for proper disposal.
<b>Uncleaned packagings:</b>	
<b>Recommendation:</b>	Disposal must be made according to official regulations.

**SECTION 14: Transport information**

<b>UN-Number</b>	
<b>ADR, IMDG, IATA</b>	UN3439
<b>14.2 UN proper shipping name</b>	
<b>ADR</b>	3439 NITRILES, TOXIC, SOLID, N.O.S. (2-Nitro-4-(trifluoromethyl)benzonitrile)
<b>IMDG, IATA</b>	NITRILES, TOXIC, SOLID, N.O.S. (2-Nitro-4-(trifluoromethyl)benzonitrile)
<b>14.3 Transport hazard class(es)</b>	
<b>ADR</b>	
	
<b>Class</b>	6.1 (T2) Toxic substances.
<b>Label</b>	6.1
<b>IMDG, IATA</b>	
	
<b>Class</b>	6.1 Toxic substances.
<b>Label</b>	6.1
<b>Packing group</b>	
<b>ADR, IMDG, IATA</b>	III

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<b>14.5 Environmental hazards:</b>	Not applicable.
<b>14.6 Special precautions for user</b> <b>Kemler Number:</b> <b>EMS Number:</b>	Warning: Toxic substances. 60 F-A,S-A
<b>14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</b>	Not applicable.
<b>Transport/Additional information:</b>	
<b>ADR</b> <b>Excepted quantities (EQ):</b> <b>Limited quantities (LQ)</b> <b>Transport category</b> <b>Tunnel restriction code</b>	E1 5 kg 2 E
<b>UN "Model Regulation":</b>	UN3439, NITRILES, TOXIC, SOLID, N.O.S. (2-Nitro-4-(trifluoromethyl) benzonitrile), 6.1, III

**SECTION 15: Regulatory information****15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture****Australian Inventory of Chemical****Substances**

Substance is not listed.

**Standard for the Uniform Scheduling of****Drugs and Poisons**

Substance is not listed.

**National regulations****Information about limitation of use:**For use only by technically qualified individuals.  
Employment restrictions concerning young persons must be observed.**Water hazard class:**

Water hazard class 1 (Self-assessment): slightly hazardous for water.

**Other regulations, limitations and prohibitive regulations****ELINCS (European List of Notified Chemical****Substances)**

Substance is not listed.

**Substances of very high concern (SVHC)****according to REACH, Article 57**

Substance is not listed.

**REACH - Pre-registered substances**

Substance is listed.

**15.2 Chemical safety assessment:**

A Chemical Safety Assessment has not been carried out.

**SECTION 16: Other information**

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

**Department issuing data specification sheet:**

Health, Safety and Environmental Department.

**Abbreviations and acronyms:**

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)  
 IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)  
 ICAO: International Civil Aviation Organization  
 ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)  
 ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)  
 IMDG: International Maritime Code for Dangerous Goods  
 IATA: International Air Transport Association  
 GHS: Globally Harmonized System of Classification and Labelling of Chemicals  
 EINECS: European Inventory of Existing Commercial Chemical Substances  
 CAS: Chemical Abstracts Service (division of the American Chemical Society)  
 LC50: Lethal concentration, 50 percent  
 LD50: Lethal dose, 50 percent

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