

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

Product name 1,2,4-Triazole-d3  
Product number 15900-4939D-100AN5  
REACH No. A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

Identified specific analytics  
uses

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

Company NEOCHEMA GmbH  
Uwe-Zeidler-Ring 10  
55294 Bodenheim, Germany  
Telephone +49 6135 933199 0  
Fax +49 6135 933199 19  
E-Mail [info@neochema.com](mailto:info@neochema.com)

**1.4 Emergency telephone number**

Emergency Phone +49 6135 933199 0  
This number is only reachable during office hours (Mo - Fr, 08:00 AM - 4:00 PM CET).

**SECTION 2: Hazards identification****2.1 Classification according to Regulation (EC) No 1272/2008**

Flam. liq. (category 2), H225  
Acute tox. (oral, category 4), H302  
Acute tox. (dermal, category 4), H312  
Acute tox. (inhalation, category 4), H332  
Eye irrit. (category 2), H319  
For the full text of the H-Statements mentioned in this Section, see Section 2.2.

**2.2 Labelling according Regulation (EC) No 1272/2008****Pictogram**

Signal word **Danger**

**Hazard statements**

H225 Highly flammable liquid and vapour.  
H319 Causes serious eye irritation.  
H302 + H312 + H332 Harmful if swallowed, in contact with skin or inhaled.

**Precautionary statements**

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.  
P233 Keep container tightly closed.  
P280 Wear protective gloves / protective clothing / eye protection / face protection  
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER / doctor.  
P302 + P352 IF ON SKIN: Wash with plenty of 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.  
P370 + P378 In case of fire: Use carbon dioxide, sand or extinguishing powder to extinguish.

**Supplemental Hazard Statements (EU)**

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.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

This product is a mixture.

### 3.2 Mixtures

Ingredient: Acetonitrile; CAS-No.: 75-05-8; EG-No.: 200-835-2; REACH-No.: 01-2119471307-38-XXXX; Classification: H225, H302, H312, H319, H332; Flam. Liq 2; Acute Tox. 4; Acute Tox. 4; Eye Irrit. 2; Acute Tox. 4; Concentration:  $\geq 90$  -  $\leq 100$  %

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

Substances listed on the 'Candidate List of Substances of Very High Concern (SVHC) for authorisation' of the European Chemical Agency (ECHA), are not intentional ingredient of this product. It is not to be expected that those substances are in quantity of  $\geq 0,1$  % in this product.

## SECTION 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.

#### If inhaled

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

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution. Consult a physician.

#### 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

## SECTION 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

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

## SECTION 6: Accidental release measures

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

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas. For personal protection see section 8.11.

**6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

**6.3 Methods and materials for containment and cleaning up**

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing or collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local regulations (see section 13).

**6.4 Reference to other sections**

For disposal see section 13.

**SECTION 7: Handling and storage****7.1 Precautions for safe handling**

Avoid exposure. Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

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

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

**7.3 Specific end uses**

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**

Ingredient: Acetonitrile; CAS-No.: 75-05-8; TWA: 40 ppm, 70 mg/m<sup>3</sup>; AGW: 10 ppm, 17 mg/m<sup>3</sup>

**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 contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

**Body Protection**

Impervious clothing, Flame retardant antistatic protective clothing., 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 respirator with multi-purpose combination (US) or type ABEK (EN 14387) 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**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

**SECTION 9: Physical and chemical properties****9.1 Information on basic physical and chemical properties**

These information refer to the main component and are literature values.

- |                                 |               |
|---------------------------------|---------------|
| a) Physical state               | clear, liquid |
| b) Color                        | colorless     |
| c) Odor                         | like ether    |
| d) Melting point/freezing point | -48 °C        |

e) Initial boiling point and boiling range	81-82 °C
f) Flammability	No Data available
g) Upper/lower flammability or explosive limits	upper: 16 %(V) ; lower: 4,4 %(V)
h) Flash point	2 °C - closed crucible
i) Autoignition temperature	No Data available
j) Decomposition temperature	No Data available
k) pH	No Data available
l) Viscosity	dynamic: 0,350 Pa.s at 20,0 °C
m) Water solubility	1 000 g/l at 25 °C completely soluble
n) Partition coefficient: n-octanol/water	log Pow: -0,54 bei 25 °C - Bioaccumulation is not expected
o) Vapor pressure	98,64 hPa at 20 °C
p) Density Relative density	0,786 g/cm <sup>3</sup> at 25 °C
q) Relative vapor density	No Data available
r) Particle characteristics	No Data available

## 9.2 Other safety information

No data available.

## SECTION 10: Stability and reactivity

These informations refer to the main component.

### 10.1 Reactivity

Vapours can form an explosive mixture with air.

### 10.2 Chemical stability

The product is chemically stable under normal ambient conditions (room temperature).

### 10.3 Possibility of hazardous reactions

Violent reactions possible with: strong bases, strong reducing agents; risk of explosion with: nitrates, nitrates, perchloric acid, concentrated sulphuric acid, with heat; risk of ignition or formation of flammable gases or vapours with: oxidising agents, nitric acid, nitrogen dioxide, with catalyst; development of dangerous gases or vapours with: acids

### 10.4 Conditions to avoid

warming

### 10.5 Incompatible materials

No Data available

### 10.6 Hazardous decomposition products

In case of fire: see Chapter 5

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

No data available for the product.

#### Acute toxicity

Ingredient: Acetonitrile; CAS-No.: 75-05-8; LD(50) (oral, mouse): 617 mg/kg; (literature); LD(50) (dermal, ATE): 1100 mg/kg; (literature); LD(50) (inhalation, ATE): 11 mg/L; (literature);

ATE-Mix (oral): 617 mg/kg

ATE-Mix (dermal): 1100 mg/kg

ATE-Mix (inhalation): 11 mg/L

#### Skin corrosion / irritation

The mixture is not classified.

#### Serious eye damage / eye irritation

The mixture causes serious eye irritation. The classification results from specific concentration limits.

**Respiratory or skin sensitisation**

The mixture is not classified.

**Germ cell mutagenicity**

The mixture is not classified.

**Carcinogenicity**

The mixture is not classified.

**Reproductive toxicity**

The mixture is not classified.

**Specific target organ toxicity – single exposure**

The mixture is not classified.

**Specific target organ toxicity – repeated exposure**

The mixture is not classified.

**Aspiration hazard**

The mixture is not classified.

**SECTION 12: Ecological information****12.1 Toxicity**

The mixture is not classified.

**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**

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.

**12.6 Other adverse effects**

No data available

**SECTION 13: Disposal considerations****13.1 Waste treatment methods****Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

**Contaminated packaging**

Dispose of as unused product.

**SECTION 14: Transport information****14.1 UN number**

ADR/RID: 1648

IMDG: 1648

IATA: 1648

**14.2 UN proper shipping name**

ADR/RID: Acetonitrile

IMDG: Acetonitrile

IATA: Acetonitrile

**14.3 Transport hazard classes**

ADR/RID: 3

IMDG: 3

IATA: 3

**14.4 Packaging group**

ADR/RID: II

IMDG: II

IATA: II

**14.5 Environmental hazards**

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

**14.6 Special precautions for user**

Tunnel restriction code (D/E)

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

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

**15.2 Chemical Safety Assessment**

For this product a chemical safety assessment was not carried out.

**SECTION 16: Other information**

## Further information

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**Full text of H-Statements referred to under section 3:**

H225 – Highly flammable liquid and vapour.

H302 – Harmful if swallowed.

H312 – Harmful in contact with skin.

H319 – Causes serious eye irritation.

H332 – Harmful if inhaled.