

**SAFETY DATA SHEET**

according to Regulation (EC) No. 1907/2006

Version 7.4

Revision Date 05.02.2025

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

Product name : Allopurinol Related Compound D

Product Number : PHR2008

Brand : Sigma-Aldrich

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration or the annual tonnage does not require a registration.

CAS-No. : 6994-25-8

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

Identified uses : Laboratory chemicals, Manufacture of substances

**1.3**

CHEMIKART

**1.4 Emergency telephone**

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

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

Acute toxicity, (Category 4) H302: Harmful if swallowed.

Eye irritation, (Category 2) H319: Causes serious eye irritation.

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

Pictogram

Signal Word Warning

Hazard Statements  
H302 Harmful if swallowed.

|                                |                                                                                                                                  |
|--------------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| H319                           | Causes serious eye irritation.                                                                                                   |
| Precautionary Statements       |                                                                                                                                  |
| P264                           | Wash skin thoroughly after handling.                                                                                             |
| P270                           | Do not eat, drink or smoke when using this product.                                                                              |
| P280                           | Wear eye protection/ face protection.                                                                                            |
| P301 + P312                    | IF SWALLOWED: 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. |
| P337 + P313                    | If eye irritation persists: Get medical advice/ attention.                                                                       |
| Supplemental Hazard Statements | none                                                                                                                             |

### Reduced Labeling (<= 125 ml)

Pictogram

|                                |         |
|--------------------------------|---------|
| Signal Word                    | Warning |
| Hazard Statements              | none    |
| Precautionary Statements       | none    |
| 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

|                  |                                                                    |
|------------------|--------------------------------------------------------------------|
| Synonyms         | : Ethyl 5-amino-1H-pyrazole-4-carboxylate (Allopurinol Impurity D) |
| Formula          | : C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>      |
| Molecular weight | : 155,16 g/mol                                                     |
| CAS-No.          | : 6994-25-8                                                        |
| EC-No.           | : 230-262-3                                                        |

| Component                                  | Classification | Concentration                        |
|--------------------------------------------|----------------|--------------------------------------|
| <b>ethyl 3-aminopyrazole-4-carboxylate</b> |                |                                      |
| CAS-No.                                    | 6994-25-8      | Acute Tox. 4; Eye Irrit. 2; <= 100 % |

|        |           |            |  |
|--------|-----------|------------|--|
| EC-No. | 230-262-3 | H302, H319 |  |
|--------|-----------|------------|--|

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

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material 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.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

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

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

### 5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## **SECTION 6: Accidental release measures**

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

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.  
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**

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### **6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

For precautions see section 2.2.

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

#### **Storage conditions**

Tightly closed. Dry.

#### **Storage class**

Storage class (TRGS 510): 11: Combustible Solids

### **7.3 Specific end use(s)**

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

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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

### **8.2 Exposure controls**

#### **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). Safety glasses

##### **Skin protection**

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 (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm  
Break through time: 480 min  
Material tested:KCL 741 Dermatril® L

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 (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested:KCL 741 Dermatril® L

### **Body Protection**

protective clothing

### **Respiratory protection**

required when dusts 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 P2

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.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

- |                                                 |                                                                               |
|-------------------------------------------------|-------------------------------------------------------------------------------|
| a) Physical state                               | powder                                                                        |
| b) Color                                        | white                                                                         |
| c) Odor                                         | No data available                                                             |
| d) Melting point/freezing point                 | Melting point/ range: 102 - 106 °C - Regulation (EC) No. 440/2008, Annex, A.1 |
| e) Initial boiling point and boiling range      | No data available                                                             |
| f) Flammability (solid, gas)                    | No data available                                                             |
| g) Upper/lower flammability or explosive limits | No data available                                                             |
| h) Flash point                                  | No data available                                                             |
| i) Autoignition temperature                     | No data available                                                             |
| j) Decomposition temperature                    | No data available                                                             |

- |                                              |                                                                                  |
|----------------------------------------------|----------------------------------------------------------------------------------|
| k) pH                                        | No data available                                                                |
| l) Viscosity                                 | Viscosity, kinematic: No data available<br>Viscosity, dynamic: No data available |
| m) Water solubility                          | at 20 °C insoluble                                                               |
| n) Partition coefficient:<br>n-octanol/water | No data available                                                                |
| o) Vapor pressure                            | No data available                                                                |
| p) Density                                   | No data available                                                                |
| Relative density                             | No data available                                                                |
| q) Relative vapor<br>density                 | No data available                                                                |
| r) Particle<br>characteristics               | No data available                                                                |
|                                              |                                                                                  |
| s) Explosive properties                      | Not classified as explosive.                                                     |
| t) Oxidizing properties                      | none                                                                             |

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

no information available

### 10.4 Conditions to avoid

no information available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - female - 573,27 mg/kg  
(OECD Test Guideline 401)

Inhalation: No data available

LD50 Dermal - Rat - male and female - > 10.000 mg/kg  
(OECD Test Guideline 402)

**Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: slight irritation

(OECD Test Guideline 405)

**Respiratory or skin sensitization**

No data available

**Germ cell mutagenicity**

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

**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

## 11.2 Additional Information

### Endocrine disrupting properties

**Product:**

Assessment

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.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Hazardous properties cannot be excluded.

Handle in accordance with good industrial hygiene and safety practice.

No data available

No data available

No data available

No data available

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.

|            |                                                                                                                                                                                                                                                               |
|------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Assessment | : 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. |
|------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

No data available

No data available

ADR/RID: -                      IMDG: -                      IATA: -

ADR/RID: Not dangerous goods  
IMDG: Not dangerous goods  
IATA: Not dangerous goods

ADR/RID: - IMDG: - IATA: -

ADR/RID: - IMDG: - IATA: -

ADR/RID: no                      IMDG Marine pollutant: no                      IATA: no



**14.6 Special precautions for user**

No data available

**Further information**

Not classified as dangerous in the meaning of transport regulations.

**14.7 Maritime transport in bulk according to IMO instruments**

Not applicable for product as supplied.

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**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.

**Other regulations**

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

**15.2 Chemical Safety Assessment**

For this product a chemical safety assessment was not carried out

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**SECTION 16: Other information****Full text of H-Statements**

|      |                                |
|------|--------------------------------|
| H302 | Harmful if swallowed.          |
| H319 | Causes serious eye irritation. |

## Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

## Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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