

## Chemical Safety Data Sheet MSDS / SDS

**4,5-DIMETHYL-2-NITROPHENYL ISOCYANATE**Revision Date:2026-05-31 Revision Number:1

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

Product name : 4,5-DIMETHYL-2-NITROPHENYL ISOCYANATE  
CBnumber : CB3293618  
CAS : 102561-40-0  
Synonyms : 1-isocyanato-4,5-dimethyl-2-nitrobenzene;4,5-DIMETHYL-2-NITROPHENYL ISOCYANATE 97%

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 010-86108875

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**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

**Precautionary statements**

P501 Dispose of contents/container to.....

P330 Rinse mouth.

P301+P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell.

P270 Do not eat, drink or smoke when using this product.

P264 Wash skin thoroughly after handling.

P501 Dispose of contents/container to.....

P363 Wash contaminated clothing before reuse.

P322 Specific measures (see ...on this label).

P312 Call a POISON CENTER or doctor/physician if you feel unwell.

P302+P352 IF ON SKIN: wash with plenty of soap and water.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P312 Call a POISON CENTER or doctor/physician if you feel unwell.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

P271 Use only outdoors or in a well-ventilated area.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P362 Take off contaminated clothing and wash before reuse.

P332+P313 IF SKIN irritation occurs: Get medical advice/attention.

P321 Specific treatment (see ... on this label).

P302+P352 IF ON SKIN: wash with plenty of soap and water.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P264 Wash skin thoroughly after handling.

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

Continuerinsing.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P264 Wash skin thoroughly after handling.

#### **Hazard statements**

H302 Harmful if swallowed

H312 Harmful in contact with skin

H332 Harmful if inhaled

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: 4,5-DIMETHYL-2-NITROPHENYL ISOCYANATE
Synonyms	: 1-isocyanato-4,5-dimethyl-2-nitrobenzene;4,5-DIMETHYL-2-NITROPHENYL ISOCYANATE 97%
CAS	: 102561-40-0
MF	: C9H8N2O3
MW	: 192.17

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## SECTION 4: First aid measures

### **General advice**

First aiders need to protect themselves. Show this safety data sheet to the doctor in attendance.

### **If inhaled**

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

### **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. 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) and/or in section 11

#### **Protection of first-aiders**

For personal protection see section 8.

#### **Notes to physician**

No data available

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## SECTION 5: Firefighting measures

#### **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.

#### **Specific hazards during fire fighting**

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

#### **Hazardous combustion products**

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

#### **Specific extinguishing methods**

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

#### **Special protective equipment 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.

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## SECTION 6: Accidental release measures

#### **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. Advice for emergency responders: 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.

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

### **Handling**

#### **Advice on safe handling**

Work under hood. Do not inhale substance/mixture.

#### **Avoidance of contact**

Strong oxidizing agents

### **Storage**

#### **Further information on storage conditions**

Tightly closed. Dry. Keep locked up or in an area accessible only to qualified or authorised persons.

#### **Storage class**

11, Combustible Solids

#### **Recommended storage temperature**

Recommended storage temperature see product label.

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

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

Contains no substances with occupational exposure limit values.

### **Engineering measures**

No data available

### **Personal protective equipment**

#### **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.

#### **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 and body protection**

protective clothing

**Hand protection**

**Material**

Nitrile rubber

**Break through time**

480 min

**Glove thickness**

0.11 mm

**Protective index**

Full contact

**Manufacturer**

KCL 741 L

**Material**

Nitrile rubber

**Break through time**

480 min

**Glove thickness**

0.11 mm

**Protective index**

Splash contact

**Manufacturer**

KCL 741 L

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

**Hygiene measures**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

powder

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**Color**

yellow

**Odor**

No data available

**Odor Threshold**

No data available

**pH**

No data available

**Melting point/ range**

85 - 89 °C

**Boiling point/boiling range**

321.6±42.0 °C(Predicted)

**Flash point**

No data available

**Evaporation rate**

No data available

**Flammability (solid, gas)**

No data available

**Flammability (liquids)**

No data available

**Burning rate**

No data available

**Upper explosion limit / Upper flammability limit**

No data available

**Lower explosion limit / Lower flammability limit**

No data available

**Vapor pressure**

No data available

**Relative vapor density**

No data available

**Relative density**

1.24±0.1 g/cm<sup>3</sup>(Predicted)

**Density**

1.24±0.1 g/cm<sup>3</sup>(Predicted)

**Water solubility**

No data available

**Partition coefficient: n-octanol/water**

No data available

#### **Autoignition temperature**

No data available

#### **Decomposition temperature**

No data available

#### **Viscosity, dynamic**

No data available

#### **Viscosity, kinematic**

No data available

#### **Flow time**

No data available

#### **Explosive properties**

No data available

#### **Oxidizing properties**

none

#### **Molecular weight**

192.17 g/mol

#### **Particle characteristics Particle size**

No data available

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## SECTION 10: Stability and reactivity

### **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.

### **Chemical stability**

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

### **Possibility of hazardous reactions**

No data available

### **Conditions to avoid**

Avoid moisture. no information available

### **Incompatible materials**

Strong oxidizing agents

## **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**

Acute toxicity estimate Oral - Expert judgement - 500.1 mg/kg

Acute toxicity estimate Inhalation - Expert judgement - 4 h - 1.5 mg/l - dust/mist

Acute toxicity estimate Dermal - Expert judgement - 1,100 mg/kg

#### **Skin corrosion/irritation**

Remarks: Causes skin irritation.

#### **Serious eye damage/eye irritation**

Remarks: Causes serious eye irritation.

#### **Respiratory or skin sensitization**

May cause allergic respiratory and skin reactions

#### **Germ cell mutagenicity**

Classified based on available data. For more details, see section 2

#### **Carcinogenicity**

Classified based on available data. For more details, see section 2

#### **Reproductive toxicity**

Classified based on available data. For more details, see section 2

#### **Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation.

#### **Specific target organ toxicity - repeated exposure**

Classified based on available data. For more details, see section 2

#### **Aspiration hazard**

Classified based on available data. For more details, see section 2

### **11.2 Additional Information**

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache,

Nausea, Vomiting, Repeated exposure may cause asthma.

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

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## **SECTION 12: Ecological information**

### **Ecotoxicity**

No data available

### **Persistence and degradability**

No data available

### **Bioaccumulative potential**

No data available

### **Mobility in soil**

No data available

### **Other adverse effects**

No data available

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## SECTION 13: Disposal considerations

### **Disposal methods**

#### **Waste from residues**

Offer surplus and non-recyclable solutions to a licensed disposal company.

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## SECTION 14: Transport information

### **International Regulations**

#### **IATA-DGR**

UN/ID No. : UN 3335

Proper shipping name : Aviation regulated solid, n.o.s.

(4,5-Dimethyl-2-nitrophenyl isocyanate)

Class : 9

Packing group : III

Labels : Class 9 - Miscellaneous dangerous substances and articles

Packing instruction (cargo aircraft) : 956

Packing instruction (passenger aircraft) : 956

#### **IMDG-Code**

UN number : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

EmS Code : Not applicable

Marine pollutant : no

### **Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code**

Not applicable for product as supplied.

## National Regulations

### JT/T 617

UN number : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

Environmentally hazardous : no

### Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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## SECTION 15: Regulatory information

Catalogue of Hazardous Chemicals : This product is not listed in the catalogue of hazardous chemicals, but it meets the definition of hazardous chemicals and its principles of determination.

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

### National regulatory information

#### Regulations on Safety Management of Hazardous Chemicals

#### Identification of Major Hazard Installations for Hazardous Chemicals (GB 18218)

Not listed

#### Hazardous Chemicals for Priority Management

Not listed under SAWS

#### Regulations on Labour Protection in Workplaces where Toxic Substances are Used

#### Catalogue of Highly Toxic Chemicals

Not listed

#### Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals

#### China Severely Restricted Toxic Chemicals for Import and Export

Not listed

#### Measures on the Environmental Administration of New Chemical Substances Registration

## Registration/Notification number

B1A222242806

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## SECTION 16: Other information

### Full text of other abbreviations

AIIIC - Australian Inventory of Industrial Chemicals

ANTT - National Agency for Transport by Land of Brazil

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)

EC<sub>x</sub> - Concentration associated with x% response

EL<sub>x</sub> - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and New Chemical Substances (Japan)

ErC<sub>x</sub> - Concentration associated with x% growth rate response

ERG - Emergency Response Guide

GHS - Globally Harmonised 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

IC<sub>50</sub> - 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 Organisation

ISHL - Industrial Safety and Health Law (Japan)

ISO - International Organisation for Standardisation

KECI - Korea Existing Chemicals Inventory

LC<sub>50</sub> - Lethal Concentration to 50 % of a test population

LD<sub>50</sub> - Lethal Dose to 50% of a test population (Median Lethal Dose)

MARPOL - International Convention for the Prevention of Pollution from Ships

MERCOSUR - The Agreement for the Facilitation of the Transport of Dangerous Goods

n.o.s. - Not Otherwise Specified

Nch - Chilean Norm

NO(A)EC - No Observed (Adverse) Effect Concentration

NO(A)EL - No Observed (Adverse) Effect Level

NOELR - No Observable Effect Loading Rate

NOM - Official Mexican Norm

NTP - National Toxicology Program

NZIoC - New Zealand Inventory of Chemicals

OECD - Organisation 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

SADT - Self-Accelerating Decomposition Temperature

SDS - Safety Data Sheet

TCSI - Taiwan Chemical Substance Inventory

TDG - Transportation of Dangerous Goods

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

WHMIS - Workplace Hazardous Materials Information System

**Disclaimer:**

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.