

## Chemical Safety Data Sheet MSDS / SDS

**2-Nitro-4-methylsulfonyltoluene**

Revision Date:2024-04-20 Revision Number:1

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

Product name : 2-Nitro-4-methylsulfonyltoluene  
CBnumber : CB5127973  
CAS : 1671-49-4  
EINECS Number : 430-550-0  
Synonyms : 2-Nitro-4-methylsulfonyltoluene

**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 : 400-158-6606

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

Acute toxicity - Category 4, Oral  
Skin sensitization, Category 1  
Reproductive toxicity, Category 2  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

**Label elements****Pictogram(s)**

☐

Signal word : Warning

**Hazard statement(s)**

H302 Harmful if swallowed  
H317 May cause an allergic skin reaction  
H361 Suspected of damaging fertility or the unborn child  
H402 Harmful to aquatic life  
H412 Harmful to aquatic life with long lasting effects

**Precautionary statement(s)**

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

P273 Avoid release to the environment.

**Prevention**

P264 Wash ... thoroughly after handling.

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

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

P272 Contaminated work clothing should not be allowed out of the workplace.

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

P203 Obtain, read and follow all safety instructions before use.

P273 Avoid release to the environment.

**Response**

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P333+P317 If skin irritation or rash occurs: Get medical help.

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

P362+P364 Take off contaminated clothing and wash it before reuse.

P318 IF exposed or concerned, get medical advice.

**Storage**

P405 Store locked up.

**Disposal**

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

**Other hazards**

no data available

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## SECTION 3: Composition/information on ingredients

**Substance**

Product name	: 2-Nitro-4-methylsulfonyltoluene
Synonyms	: 2-Nitro-4-methylsulfonyltoluene
CAS	: 1671-49-4
EC number	: 430-550-0
MF	: C <sub>8</sub> H <sub>9</sub> NO <sub>4</sub> S
MW	: 215.23

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## SECTION 4: First aid measures

**Description of first aid measures**

#### If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

#### Following skin contact

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

#### Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

#### Most important symptoms and effects, both acute and delayed

no data available

#### Indication of any immediate medical attention and special treatment needed

no data available

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## SECTION 5: Firefighting measures

#### Extinguishing media

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

#### Specific Hazards Arising from the Chemical

no data available

#### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### NFPA 704



■ HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

■ FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

□ SPEC.

## SECTION 6: Accidental release measures

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

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### **Environmental precautions**

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

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

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

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## SECTION 7: Handling and storage

### **Precautions for safe handling**

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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## SECTION 8: Exposure controls/personal protection

### **Control parameters**

#### **Occupational Exposure limit values**

no data available

#### **Biological limit values**

no data available

### **Exposure controls**

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

### **Individual protection measures**

#### **Eye/face protection**

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

### Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. 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.

### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

### Thermal hazards

no data available

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Physical state	Solid. Powder.
Colour	White.
Odour	no data available
Melting point/freezing point	115.25 °C. Atm. press.:Ca. 1. Remarks:Assumed ambient atmospheric pressure.
Boiling point or initial boiling point and boiling range	Atm. press.:Ca. 1 atm. Remarks:Pressure assumed to be ambient atmospheric.
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	188.3°C
Auto-ignition temperature	> 116 °C. Remarks:No ignition detected up to the melting point. Ambient atmospheric pressure.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	In water: 370 mg/L. Temperature:25 °C. pH:1.73.
Partition coefficient n-octanol/water	log Pow = 0.93. Temperature:20 °C.
Vapour pressure	0 Pa. Temperature:25 °C. Remarks:Extrapolated.
Density and/or relative density	1.48. Temperature:20 °C.
Relative vapour density	no data available
Particle characteristics	no data available

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## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

no data available

### Possibility of hazardous reactions

no data available

**Conditions to avoid**

no data available

**Incompatible materials**

no data available

**Hazardous decomposition products**

no data available

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**SECTION 11: Toxicological information****Acute toxicity**

- Oral: LD50 - rat (male) - 1 426 mg/kg bw.
- Inhalation: LC50 - rat (male/female) - > 5.41 mg/L air.
- Dermal: LD50 - rat (male/female) - > 2 000 mg/kg bw.

**Skin corrosion/irritation**

no data available

**Serious eye damage/irritation**

no data available

**Respiratory or skin sensitization**

no data available

**Germ cell mutagenicity**

no data available

**Carcinogenicity**

no data available

**Reproductive toxicity**

no data available

**STOT-single exposure**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

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## SECTION 12: Ecological information

### Toxicity

Toxicity to fish: LC50 - *Oncorhynchus mykiss* (previous name: *Salmo gairdneri*) - 59 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 120 mg/L - 48 h.

Toxicity to algae: EC50 - *Pseudokirchneriella subcapitata* (previous names: *Raphidocelis subcapitata*, *Selenastrum capricornutum*) - 16 mg/L - 72 h.

Toxicity to microorganisms: EC50 - *Pseudomonas putida* - > 32 mg/L - 6 h.

### 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

#### Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

#### Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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## SECTION 14: Transport information

### UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Transport hazard class(es)**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Packing group, if applicable**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Environmental hazards**

ADR/RID: No

IMDG: No

IATA: No

### **Special precautions for user**

no data available

### **Transport in bulk according to IMO instruments**

no data available

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## SECTION 15: Regulatory information

### **Safety, health and environmental regulations specific for the product in question**

#### **European Inventory of Existing Commercial Chemical Substances (EINECS)**

Not Listed.

#### **EC Inventory**

Not Listed.

#### **United States Toxic Substances Control Act (TSCA) Inventory**

Not Listed.

#### **China Catalog of Hazardous chemicals 2015**

Not Listed.

#### **New Zealand Inventory of Chemicals (NZIoC)**

Not Listed.

#### **PICCS**

Not Listed.

#### **Vietnam National Chemical Inventory**

Not Listed.

#### **IECSC**

Listed.

#### **Korea Existing Chemicals List (KECL)**

Not Listed.



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## SECTION 16: Other information

### Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

### References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: [http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

#### 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.