

Chemical Safety Data Sheet MSDS / SDS

5-Methyl-2-[(2-nitrophenyl)amino]thiophene-3-carbonitrile

Revision Date:2025-07-26 Revision Number:1

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

Product name : 5-Methyl-2-[(2-nitrophenyl)amino]thiophene-3-carbonitrile
CBnumber : CB3163423
CAS : 138564-59-7
EINECS Number : 421-300-1
Synonyms : ROY,OLANZAPINE RELATED COMPOUND A

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

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

Eye irritation, Category 2
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

Label elements**Pictogram(s)**

☐

Signal word : Warning

Hazard statement(s)

H319 Causes serious eye irritation
H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

P273 Avoid release to the environment.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.
Continuerinsing.

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

Prevention

P264 Wash ... thoroughly after handling.

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

P273 Avoid release to the environment.

Response

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

P391 Collect spillage.

Storage

none

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

SECTION 3: Composition/information on ingredients

Substance

Product name	: 5-Methyl-2-[(2-nitrophenyl)amino]thiophene-3-carbonitrile
Synonyms	: ROY,OLANZAPINE RELATED COMPOUND A
CAS	: 138564-59-7
EC number	: 421-300-1
MF	: C ₁₂ H ₉ N ₃ O ₂ S
MW	: 259.28

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

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.

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.

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.

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/flamm 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

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	neat
Colour	no data available
Odour	no data available
Melting point/freezing point	≥ 109 - ≤ 111 °C. Atm. press.:Ca. 1 atm.
Boiling point or initial boiling point and boiling range	Atm. press.:Ca. 1 atm. Remarks:Not determinable.
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	63°C(lit.)
Auto-ignition temperature	Remarks:No self-ignition observed up to the melting point.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	In water: 1.397 ug/ml. Temperature:20 °C. pH:Ca. 6.04. Remarks:Test substance in water.;1.496 ug/ml. Temperature:20 °C. pH:Ca. 4.;1.427 ug/ml. Temperature:20 °C. pH:Ca. 7.

Partition coefficient n-octanol/water	log Pow = 3.2. Remarks:PH & temp not available on report.
Vapour pressure	Ca. 0 Pa. Temperature:Ca. 25 °C.;Remarks:Not determinable.;Remarks:Not determinable.
Density and/or relative density	Ca. 1.467 g/cm3. Temperature:20 °C.
Relative vapour density	no data available
Particle characteristics	no data available

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

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: LD50 - (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

SECTION 12: Ecological information

Toxicity

Toxicity to fish: Median lethal concentration - *Oncorhynchus mykiss* (previous name: *Salmo gairdneri*) - 1 279 µg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - ≥ 274 - ≤ 370 µg/L - 48 h.

Toxicity to algae: EC50 - *Selenastrum capricornutum* - ca. 458 µg/L - 3 d.

Toxicity to microorganisms: Inhibitory Effect - activated sludge of a predominantly domestic sewage - $\geq 1\,198.08$ µg/L - 3 h. Remarks: Not a respiratory inhibitor.

Persistence and degradability

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

Other adverse effects

no data available

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.

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: Yes

IMDG: Yes

IATA: Yes

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

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

Not Listed.

Korea Existing Chemicals List (KECL)

Not Listed.

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

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/>

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