

Chemical Safety Data Sheet MSDS / SDS

5-tert-butyl-2,4,6-trinitro-m-xylene SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: 5-tert-butyl-2,4,6-trinitro-m-xylene

CAS: 81-15-2

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.in

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SECTION 2: Hazards identification**Classification of the substance or mixture**Explosives, Division 1.1
Carcinogenicity, Category 2

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

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H201 Explosive; mass explosion hazard
H351 Suspected of causing cancer
H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P230 Keep wetted with ...
P234 Keep only in original packaging.
P240 Ground and bond container and receiving equipment.
P250 Do not subject to grinding/shock/friction/....
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

P370+P372+P380+P373 In case of fire: Explosion risk. Evacuate area. DO NOT fight fire when fire reaches explosives.
P318 IF exposed or concerned, get medical advice.
P391 Collect spillage.

Storage

P401 Store in accordance with...
P405 Store locked up.

Disposal

P503 Refer to manufacturer/supplier... for information on disposal/recovery/recycling.

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 which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name: 5-tert-butyl-2,4,6-trinitro-m-xylene

Common names and synonyms: 5-tert-butyl-2,4,6-trinitro-m-xylene

CAS number: 81-15-2

EC number: 201-329-4

Concentration: 100%

SECTION 4: First aid measures

Description of necessary 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/effects, acute and delayed

Excerpt from ERG Guide 149 [Substances (Self-Reactive)]: Inhalation or contact with vapors, substance or decomposition products may cause severe injury or death. May produce irritating, toxic and/or corrosive gases. Runoff from fire control may cause pollution. (ERG, 2016)

Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Aromatic hydrocarbons and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

If material on fire or involved in fire: Use water in flooding quantities as fog. Solid streams of water may spread fire. Use foam, dry chemical, or carbon dioxide. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Keep run-off water out of sewers and water sources.

Specific hazards arising from the chemical

Excerpt from ERG Guide 149 [Substances (Self-Reactive)]: Self-decomposition, self-polymerization, or self-ignition may be triggered by heat, chemical reaction, friction or impact. May be ignited by heat, sparks or flames. Some may decompose explosively when heated or involved in a fire. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. May burn violently. Decomposition or polymerization may be self-accelerating and produce large amounts of gases. Vapors or dust may form explosive mixtures with air. (ERG, 2016)

Special protective actions for fire-fighters

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

SRP: Wastewater from contaminant suppression, cleaning of protective clothing/equipment, or contaminated sites should be contained and evaluated for subject chemical or decomposition product concentrations. Concentrations shall be lower than applicable environmental discharge or disposal criteria. Alternatively, pretreatment and/or discharge to a POTW is acceptable only after review by the governing authority. Due consideration shall be given to remediation worker exposure (inhalation, dermal and ingestion) as well as fate during treatment, transfer and disposal. If it is not practicable to manage the chemical in this fashion, it must meet Hazardous Material Criteria for disposal.

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

Appropriate engineering 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, such as personal protective equipment (PPE)

Eye/face protection

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

Skin protection

Wear fire/flare 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 and safety characteristics

Physical state:	5-tert-Butyl-2,4,6-trinitro-m-xylene is a white to light-colored crystalline solid. It is insoluble in water and denser than water. Hence sinks in water. Contact may irritate skin, eyes, and mucous membranes. May be toxic by ingestion. Used to make other chemicals.
Colour:	Plates, needles from alcohol
Odour:	Sweet, musky odor
Melting point/freezing point:	235.4°C
Boiling point or initial boiling point and boiling range:	392.3°Cat 760 mmHg

Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	174.2°C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	Henry's Law constant = 7.73×10^{-9} atm-cu m/mol at 25 deg C (est)
Solubility:	Slightly soluble in ethanol; soluble in ethyl ether, chloroform
Partition coefficient n-octanol/water:	log Kow = 4.4
Vapour pressure:	6.35×10^{-7} mm Hg at 25 deg C (est)
Density and/or relative density:	1.325 g/cm ³
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Highly flammable. Insoluble in water.

Chemical stability

no data available

Possibility of hazardous reactions

A flammable solid. Self-decomposition or self-ignition may be triggered by heat, chemical reaction, friction or impact.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits toxic fumes of NO_x.

SECTION 11: Toxicological information**Acute toxicity**

Oral: LD50 Mouse oral 4 g/kg

Inhalation: no data available

Dermal: no data available

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: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Musk xylene, present at 100 mg/L, reached 2% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI I test(1).

Bioaccumulative potential

A BCF of 1,600 was measured in fish for musk xylene using bluegill sunfish (*Lepomis macrochirus*) which were exposed over a 16-day period(1) to water concentrations from 5 to 47 ug/L. Bioconcentration factors of 1,400-6,740 and 640-5,820 were measured for musk xylene in fish in flow-through tests using carp (*Cyprinus carpio*) with a 10 week uptake period and water concentrations of 1 ug/L and 10 ug/L respectively(2). A BCF of 3,250-6,810 was measured in fish for musk xylene using carp (*Cyprinus carpio*) which were exposed over a 12 week period to a water concentration of 1 ug/L(3). According to a classification scheme(4), these BCF values suggest the potential for bioconcentration in aquatic organisms is very high, provided the compound is not metabolized by the organism(SRC).

Mobility in soil

The Koc of musk xylene is estimated as 6,300(SRC), using a log Kow of 4.4(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that Musk xylene is expected to be immobile in soil.

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: UN2956 (For reference only, please check.)

IMDG: UN2956 (For reference only, please check.)

IATA: UN2956 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: 5-tert-BUTYL-2,4,6-TRINITRO-m- XYLENE (MUSK XYLENE) (For reference only, please check.)

IMDG: 5-tert-BUTYL-2,4,6-TRINITRO-m- XYLENE (MUSK XYLENE) (For reference only, please check.)

IATA: 5-tert-BUTYL-2,4,6-TRINITRO-m- XYLENE (MUSK XYLENE) (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 4.1 (For reference only, please check.)

IMDG: 4.1 (For reference only, please check.)

IATA: 4.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: III (For reference only, please check.)

IMDG: III (For reference only, please check.)

IATA: III (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)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

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/>

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any