ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

1,2,3-Trimethylbenzene

Revision Date:2025-02-01 Revision Number:1

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

Product identifier

Product name	: 1,2,3-Trimethylbenzene
CBnumber	: CB6853732
CAS	: 526-73-8
EINECS Number	: 208-394-8
Synonyms	: 1,2,3-trimethylbenzene,benzene,1,2,3-trimethyl-

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

Flammable liquids, Category 3

Skin irritation, Category 2

Eye irritation, Category 2

Label elements

Pictogram(s)

Signal word	Warning

Hazard statement(s)

H226 Flammable liquid and vapour

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

Precautionary statement(s)

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

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

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P233 Keep container tightly closed.

P240 Ground and bond container and receiving equipment.

P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.

P242 Use non-sparking tools.

P243 Take action to prevent static discharges.

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

P264 Wash ... thoroughly after handling.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].

P370+P378 In case of fire: Use ... to extinguish.

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

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

P332+P317 If skin irritation occurs: Get medical help.

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

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

Storage

P403+P235 Store in a well-ventilated place. Keep cool.

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	: 1,2,3-Trimethylbenzene
Synonyms	: 1,2,3-trimethylbenzene,benzene,1,2,3-trimethyl-
CAS	: 526-73-8
EC number	: 208-394-8
MF	: C9H12
MW	: 120.19

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Rinse skin with plenty of water or shower.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Do NOT induce vomiting. Refer for medical attention .

Most important symptoms and effects, both acute and delayed

no data available

Indication of any immediate medical attention and special treatment needed

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

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SECTION 5: Firefighting measures

Extinguishing media

This chemical is a flammable liquid. Poisonous gases are produced in fire. Small fires: dry chemical, carbon dioxide, water spray, or alcohol-resistant foam. Large fires: water spray, fog, or alcohol foam. Move container from fire if you can do so without risk. Spray cooling water on containers that are exposed to flames until well after fire is out. For massive fire in cargo area, use unmanned hose holder or monitoring nozzles; if this is impossible, withdraw from area and let fire burn. Isolate for one-half mile in all directions if tank car or truck is involved in fire. Vapors are heavier than air and will collect in low areas. Vapors may travel long distances to ignition sources and flashback. Vapors in confined areas may explode when exposed to fire. Containers may explode in fire. Storage containers and parts of containers may rocket great distances, in many directions. If material or contaminated runoff enters waterways, notify downstream users of potentially contaminated waters. Notify local health and fire officials and pollution control agencies. From a secure, explosion-proof location, use water spray to cool exposed containers. If cooling streams are ineffective (venting sound increases in volume and pitch, tank discolors, or shows any signs of deforming), withdraw immediately to a secure position. If employees are expected to fight fires, they must be trained and equipped in OSHA 1910.156. Trimethyl benzenes

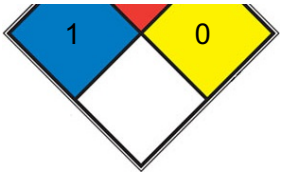
Specific Hazards Arising from the Chemical

Flammable. Above 44°C explosive vapour/air mixtures may be formed.

Advice for firefighters

Use alcohol-resistant foam, foam, powder, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

NFPA 704



■	HEALTH	1	Exposure would cause irritation with only minor residual injury (e.g. acetone, sodium bromate, potassium chloride)
■	FIRE	2	Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, sulfur)
■	REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,N2)
□	SPEC. HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Collect leaking and spilled liquid in covered containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer.

Environmental precautions

Collect leaking and spilled liquid in covered containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer.

Methods and materials for containment and cleaning up

Evacuate and restrict persons not wearing protective equipment from area of spill or leak until cleanup is complete. Remove all ignition sources. Establish forced ventilation to keep levels below explosive limit. Absorb liquids in vermiculite, dry sand, earth, peat, carbon, or similar material and deposit in sealed containers. Keep this chemical out of a confined space ... because of the possibility of an explosion ... It may be necessary to contain and dispose of this chemical as a hazardous waste. If material or contaminated runoff enters waterways, notify downstream users of potentially contaminated waters. Contact your Department of Environmental Protection or your regional office of the federal EPA for specific recommendations. If employees are required to clean up spills, they must be properly trained and equipped. OSHA 1910.120(q) may be applicable. Trimethyl benzenes

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Above 44°C use a closed system, ventilation and explosion-proof electrical equipment. Prevent build-up of electrostatic charges (e.g., by grounding). 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

Fireproof. Well closed. Separated from oxidants.Prior to working with this chemical you should be trained on its proper handling and storage. Before entering a confined space where this chemical may be present, check to make sure that an explosive concentration does not exist.

Trimethylbenzene must be stored to avoid contact with oxidizers (such as perchlorates, peroxides, permanganates, chlorates, and nitrates), and strong oxidizers (such as chlorine, bromine, and fluorine) since violent reactions occur. Store in tightly closed containers in a cool, well-ventilated area away from heat. Sources of ignition such as smoking and open flames are prohibited where this chemical is used, handled, or stored in a manner that could create a potential fire or explosion hazard. Metal containers involving the transfer of 5 gallons or more of this chemical should be grounded and bonded. Drums must be equipped with self-closing valves, pressure vacuum bungs, and flame arresters. Use only nonsparking tools and equipment, especially when opening and closing containers of this chemical. Trimethyl benzenes

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SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

EU-OEL: 100 mg/m3, 20 ppm as TWA.MAK: 100 mg/m3, 20 ppm; peak limitation category: II(2); pregnancy risk group: C

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 safety spectacles.

Skin protection

Protective gloves.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	neat
Colour	Colorless liquid
Odour	Distinctive, aromatic odor
Melting point/freezing point	271°C(lit.)
Boiling point or initial boiling point and boiling range	176°C
Flammability	Flammable Liquid
Lower and upper explosion limit/flammability limit	Lower flammable limit: 0.8% by volume; Upper flammable limit: 6.6% by volume
Flash point	44°C(lit.)

Auto-ignition temperature	878 deg F (470 deg C)
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	Soluble in acetone, alcohol, benzene, and ether (Weast, 1986)
Partition coefficient n-octanol/water	log Kow = 3.66
Vapour pressure	3.4 mm Hg (37.7 °C)
Density and/or relative density	0.894
Relative vapour density	4.15 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts with oxidants. This generates fire and explosion hazard.

Decomposes on burning. This produces toxic and irritating fumes. Reacts violently with strong oxidants. This generates fire and explosion hazard.

Chemical stability

no data available

Possibility of hazardous reactions

Reacts with oxidants. This generates fire and explosion hazard.

Conditions to avoid

no data available

Incompatible materials

Oxidizers (perchlorates, peroxides, permanganates, chlorates, nitrates), strong oxidizers (chlorine, bromine, fluorine), and nitric acid. Trimethyl benzenes

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- 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

Result:This chemical slightly increased incidences of structural chromosomal aberrations with an exogeneous metabolic activation system.

Clear reproducibility was obtained the confirmation study.

Metabolic activation: with and without metabolic activation

Method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan)

Test system: Chinese hamster lung (CHL) cells

Test Type: Chromosome aberration test in vitro

Result:Negative

Metabolic activation: with and without metabolic activation

Method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan)

Test system: Salmonella typhimurium TA100, TA1535, TA98, TA1537, E. coli WP2 uvrA

Test Type: Ames test

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes, skin and respiratory tract. The substance may cause effects on the central nervous system. If this liquid is swallowed, aspiration into the lungs may result in chemical pneumonitis.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20°C.

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: 1,2,3-Trimethylbenzene, present at 100 mg/L, reached 0% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L and the Japanese MITI test(1). 1,2,3-Trimethylbenzene had a 99(2) and 100%(3) removal in acclimated sludge and activated sludge, respectively. The concentration of 1,2,3-trimethylbenzene was reduced from 4.24 mg/L to 0.0 mg/L in 25 days at 30 deg C using a sewage inocculum(4). Biodegradation of 1,2,3-trimethylbenzene was classified as moderate in a marine environment(5). 1,2,3-Trimethylbenzene was reduced to zero in 23 days in sewage using a natural microbial flora with aeration and was reduced without aeration(6).

Bioaccumulative potential

The BCF of 1,2,3-trimethylbenzene was 133-217 at a concentration of 150 ppb and 136-259 at a concentration of 15 ppb using carp (Cypinus carpio) which were exposed over an 8-week period(1). According to a classification scheme(2), these BCFs suggest bioconcentration in aquatic organisms is high(SRC).

Mobility in soil

1,2,3-Trimethylbenzene has measured log Koc values of 3.04(1) and 2.80(2-5). These values correspond to Koc values of 1,096 and 630. 1,2,3-Trimethylbenzene also has a reported log Kom value of 2.80(6-7). According to a classification scheme(8), these Koc values suggest that 1,2,3-trimethylbenzene is expected to have low mobility in soil(SRC).

Toxics Screening Level

The acute initial threshold screening level (ITSL) for all trimethylbenzene (TMB) isomers combined is 1200 µg/m3 with 8-hr averaging time.

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: UN3295 (For reference only, please check.)

IMDG: UN3295 (For reference only, please check.)

IATA: UN3295 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: HYDROCARBONS, LIQUID, N.O.S. (For reference only, please check.)

IMDG: HYDROCARBONS, LIQUID, N.O.S. (For reference only, please check.)

IATA: HYDROCARBONS, LIQUID, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)

IMDG: 3 (For reference only, please check.)

IATA: 3 (For reference only, please check.)

Packing group, if applicable

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

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

IATA: I (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

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/

Other Information

Use of alcoholic beverages enhances the harmful effect.See ICSCs 1155 and 1389.