



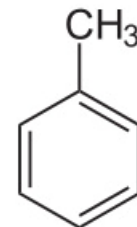
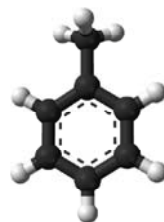
TOLUENE

Chemical Formula: C_7H_8

CAS Registry Number: 108-88-3

Molecular Weight: 92.14

PRODUCT INFORMATION



Synonyms:

- 1-Methylbenzene
- Antisal 1a
- Benzene, methyl
- Benzene, methyl-
- Benzene,methyl
- CP 25
- CP 25 (solvent)
- Methacide
- METHYL BENZENE
- Methylbenzene
- Methylbenzol
- NSC 406333
- Phenylmethane
- TOLOULE OR TOLUOL
- Toluene
- toluene
- Toluene
- tolueno
- Toluol
- Toluol
- Toulene
- UN 1294
- UN 1294

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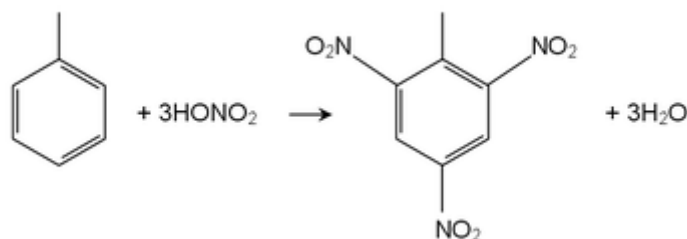


Toluene, also known as **methylbenzene**, or **Toluol**, is a clear water-insoluble liquid with the typical smell of paint thinners. Chemically it is mono-substituted benzene derivative (benzene derivative in which one hydrogen atom from the benzene molecule has been replaced by a univalent group; in this case CH₃).

It is an aromatic hydrocarbon that is widely used as an industrial feedstock and as a solvent. Like other solvents, toluene is also used as an inhalant drug for its intoxicating properties; however, this causes severe neurological harm.

Chemical properties

Toluene reacts as a normal aromatic hydrocarbon towards electrophilic aromatic substitution. The methyl group makes it around 25 times more reactive than benzene in such reactions. It undergoes smooth sulfonation to give *p*-toluenesulfonic acid, and chlorination by Cl₂ in the presence of FeCl₃ to give ortho and para isomers of chlorotoluene. It undergoes nitration to give ortho and para nitrotoluene isomers, but if heated it can give dinitrotoluene and ultimately the explosive trinitrotoluene (TNT).



With other reagents the methyl side chain in toluene may react, undergoing oxidation. Reaction with potassium permanganate leads to benzoic acid, whereas reaction with chromyl chloride leads to benzaldehyde (Étard reaction). Halogenation can be performed under free radical conditions. For example, *N*-bromosuccinimide (NBS) heated with toluene in the presence of AIBN leads to benzyl bromide. Toluene can also be treated with elemental bromine in the presence of UV light (direct sunlight) to yield benzyl bromide.

Catalytic hydrogenation of toluene to methylcyclohexane requires a high pressure of hydrogen to go to completion, because of the stability of the aromatic system. pK_a is approximately 45.

Appearance: Clear, colorless liquid.

Odor: Aromatic benzene-like.

Solubility: 0.05 gm/100gm water @ 20°C (68°F).

Specific Gravity: 0.86 @ 20°C / 4°C

pH: No information found.

% Volatiles by volume @ 21°C (70°F): 100

Boiling Point: 111°C (232°F)

Melting Point: -95°C (-139°F)

Vapor Density (Air=1): 3.14

Vapor Pressure (mm Hg): 22 @ 20°C (68°F)

Evaporation Rate (BuAc=1): 2.24



Stability and Reactivity

Stability:

Stable under ordinary conditions of use and storage. Containers may burst when heated.

Hazardous Decomposition Products:

Carbon dioxide and carbon monoxide may form when heated to decomposition.

Hazardous Polymerization:

Will not occur.

Incompatibilities:

Heat, flame, strong oxidizers, nitric and sulfuric acids, chlorine, nitrogen tetroxide; will attack some forms of plastics, rubber, coatings.

Conditions to Avoid:

Heat, flames, ignition sources and incompatibles.

Hazards Identification

Emergency Overview

POISON! DANGER! HARMFUL OR FATAL IF SWALLOWED. HARMFUL IF INHALED OR ABSORBED THROUGH SKIN. VAPOR HARMFUL. FLAMMABLE LIQUID AND VAPOR. MAY AFFECT LIVER, KIDNEYS, BLOOD SYSTEM, OR CENTRAL NERVOUS SYSTEM. CAUSES IRRITATION TO SKIN, EYES AND RESPIRATORY TRACT.

Health Rating: 2 - Moderate (Life)

Flammability Rating: 3 - Severe (Flammable)

Reactivity Rating: 1 - Slight

Contact Rating: 3 - Severe (Life)

Lab Protective Equip: GOGGLES & SHIELD; LAB COAT & APRON; VENT HOOD; PROPER GLOVES; CLASS B EXTINGUISHER

Storage Color Code: Red (Flammable)

Potential Health Effects

Inhalation:

Inhalation may cause irritation of the upper respiratory tract. Symptoms of overexposure may include fatigue, confusion, headache, dizziness and drowsiness. Peculiar skin sensations (e. g. pins and needles) or numbness may be produced. Very high concentrations may cause unconsciousness and death.

Ingestion:

Swallowing may cause abdominal spasms and other symptoms that parallel over-exposure from inhalation. Aspiration of material into the lungs can cause chemical pneumonitis, which may be fatal.

Skin Contact:

Causes irritation. May be absorbed through skin.

Eye Contact:

Causes severe eye irritation with redness and pain.

Chronic Exposure:

Reports of chronic poisoning describe anemia, decreased blood cell count and bone marrow hypoplasia. Liver and kidney damage may occur. Repeated or prolonged contact has a defatting action, causing drying, redness, dermatitis. Exposure to toluene may affect the developing fetus.

Aggravation of Pre-existing Conditions:



Persons with pre-existing skin disorders or impaired liver or kidney function may be more susceptible to the effects of this substance. Alcoholic beverage consumption can enhance the toxic effects of this substance.

First Aid Measures

Inhalation:

If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. CALL A PHYSICIAN IMMEDIATELY.

Ingestion:

Aspiration hazard. If swallowed, DO NOT INDUCE VOMITING. Give large quantities of water. Never give anything by mouth to an unconscious person. Get medical attention immediately. If vomiting occurs, keep head below hips to prevent aspiration into lungs.

Skin Contact:

In case of contact, immediately flush skin with plenty of soap and water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Call a physician immediately.

Eye Contact:

Immediately flush eyes with plenty of water for at least 15 minutes, lifting lower and upper eyelids occasionally. Get medical attention immediately.

Fire Fighting Measures

Fire:

Flash point: 7C (45F) CC

Autoignition temperature: 422C (792F)

Flammable limits in air % by volume:

l_{el}: 1.1; u_{el}: 7.1

Flammable liquid and vapor!

Dangerous fire hazard when exposed to heat or flame. Vapors can flow along surfaces to distant ignition source and flash back.

Explosion:

Above flash point, vapor-air mixtures are explosive within flammable limits noted above. Contact with strong oxidizers may cause fire or explosion. Sensitive to static discharge.

Fire Extinguishing Media:

Dry chemical, foam or carbon dioxide. Water may be used to flush spills away from exposures and to dilute spills to non-flammable mixtures.

Special Information:

In the event of a fire, wear full protective clothing and NIOSH-approved self-contained breathing apparatus with full facepiece operated in the pressure demand or other positive pressure mode. Water spray may be used to keep fire exposed containers cool.

Accidental Release Measures

Ventilate area of leak or spill. Remove all sources of ignition. Wear appropriate personal protective equipment as specified in Section 8. Isolate hazard area. Keep unnecessary and unprotected personnel from entering. Contain and recover liquid when possible. Use non-sparking tools and equipment. Collect liquid in an appropriate container



or absorb with an inert material (e. g., vermiculite, dry sand, earth), and place in a chemical waste container. Do not use combustible materials, such as saw dust. Do not flush to sewer! If a leak or spill has not ignited, use water spray to disperse the vapors, to protect personnel attempting to stop leak, and to flush spills away from exposures.

Handling and Storage

Protect against physical damage. Store in a cool, dry well-ventilated location, away from any area where the fire hazard may be acute. Outside or detached storage is preferred. Separate from incompatibles. Containers should be bonded and grounded for transfers to avoid static sparks. Storage and use areas should be No Smoking areas. Use non-sparking type tools and equipment, including explosion proof ventilation. Containers of this material may be hazardous when empty since they retain product residues (vapors, liquid); observe all warnings and precautions listed for the product.

Exposure Controls/Personal Protection

Airborne Exposure Limits:

Toluene:

- OSHA Permissible Exposure Limit (PEL):

200 ppm (TWA); 300 ppm (acceptable ceiling conc.); 500 ppm (maximum conc.).

- ACGIH Threshold Limit Value (TLV):

20 ppm (TWA), A4 - Not Classifiable as a Human Carcinogen.

Ventilation System:

A system of local and/or general exhaust is recommended to keep employee exposures below the Airborne Exposure Limits. Local exhaust ventilation is generally preferred because it can control the emissions of the contaminant at its source, preventing dispersion of it into the general work area. Please refer to the ACGIH document, *Industrial Ventilation, A Manual of Recommended Practices*, most recent edition, for details.

Personal Respirators (NIOSH Approved):

If the exposure limit is exceeded and engineering controls are not feasible, a half-face organic vapor respirator may be worn for up to ten times the exposure limit, or the maximum use concentration specified by the appropriate regulatory agency or respirator supplier, whichever is lowest. A full-face piece organic vapor respirator may be worn up to 50 times the exposure limit, or the maximum use concentration specified by the appropriate regulatory agency or respirator supplier, whichever is lowest. For emergencies or instances where the exposure levels are not known, use a full-face piece positive-pressure, air-supplied respirator. WARNING: Air-purifying respirators do not protect workers in oxygen-deficient atmospheres.

Skin Protection:

Wear impervious protective clothing, including boots, gloves, lab coat, apron or coveralls, as appropriate, to prevent skin contact.

Eye Protection:

Use chemical safety goggles and/or a full face shield where splashing is possible. Maintain eye wash fountain and quick-drench facilities in work area.



Ecological Information

Environmental Fate:

When released into the soil, this material may evaporate to a moderate extent. When released into the soil, this material is expected to leach into groundwater. When released into the soil, this material may biodegrade to a moderate extent. When released into water, this material may evaporate to a moderate extent. When released into water, this material may biodegrade to a moderate extent. When released into the air, this material may be moderately degraded by reaction with photochemically produced hydroxyl radicals. When released into the air, this material is expected to have a half-life of less than 1 day. This material is not expected to significantly bioaccumulate. This material has a log octanol-water partition coefficient of less than 3.0. Bioconcentration factor = 13.2 (eels).

Environmental Toxicity:

This material is expected to be toxic to aquatic life. The LC50/96-hour values for fish are between 10 and 100 mg/l.

Other Information

NFPA Ratings: Health: 2 Flammability: 3 Reactivity: 0

Label Hazard Warning:

POISON! DANGER! HARMFUL OR FATAL IF SWALLOWED. HARMFUL IF INHALED OR ABSORBED THROUGH SKIN. VAPOR HARMFUL. FLAMMABLE LIQUID AND VAPOR. MAY AFFECT LIVER, KIDNEYS, BLOOD SYSTEM, OR CENTRAL NERVOUS SYSTEM. CAUSES IRRITATION TO SKIN, EYES AND RESPIRATORY TRACT.

Label Precautions:

Keep away from heat, sparks and flame.
Keep container closed.
Use only with adequate ventilation.
Wash thoroughly after handling.
Avoid breathing vapor.
Avoid contact with eyes, skin and clothing.

Label First Aid:

Aspiration hazard. If swallowed, DO NOT INDUCE VOMITING. Give large quantities of water. Never give anything by mouth to an unconscious person. If vomiting occurs, keep head below hips to prevent aspiration into lungs. If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. In case of contact, immediately flush eyes or skin with plenty of water for at least 15 minutes. Remove contaminated clothing and shoes. Wash clothing before reuse. In all cases call a physician immediately.

Uses

Toluene is a common solvent, able to dissolve paints, paint thinners, silicone sealants, many chemical reactants, rubber, printing ink, adhesives (glues), lacquers, leather tanners, and disinfectants. It can also be used as a fullerene indicator, and is a raw material for toluene diisocyanate (used in the manufacture of polyurethane foam) and TNT. It is also used as a cement for fine polystyrene kits (by dissolving and then fusing surfaces) as it can be applied very precisely by brush and contains none of the bulk of an adhesive.

Industrial uses of toluene include dealkylation to benzene, and the disproportionation to a mixture of benzene and xylene in the BTX process. When oxidized it yields benzaldehyde and benzoic acid, two important



intermediates in chemistry. It is also used as a carbon source for making Multi-Wall Carbon Nanotubes. Toluene can be used to break open red blood cells in order to extract hemoglobin in biochemistry experiments.

Toluene can be used as an octane booster in gasoline fuels used in internal combustion engines. Toluene at 86% by volume fueled all the turbo Formula 1 teams in the 1980s, first pioneered by the Honda team. The remaining 14% was a "filler" of n-heptane, to reduce the octane to meet Formula 1 fuel restrictions. Toluene at 100% can be used as a fuel for both two-stroke and four-stroke engines; however, due to the density of the fuel and other factors, the fuel does not vaporize easily unless preheated to 70 degrees Celsius (Honda accomplished this in their Formula 1 cars by routing the fuel lines through the muffler system to heat the fuel). Toluene also poses similar problems as alcohol fuels, as it eats through standard rubber fuel lines and has no lubricating properties as standard gasoline does, which can break down fuel pumps and cause upper cylinder bore wear.

In Australia, toluene has been found to have been illegally combined with petrol in fuel outlets for sale as standard vehicular fuel. Toluene attracts no fuel excise, while other fuels are taxed at over 40%, so fuel suppliers are able to profit from substituting the cheaper toluene for petrol. This substitution is likely to affect engine performance and result in additional wear and tear. The extent of toluene substitution has not been determined.

Toluene has also been used as a coolant for its good heat transfer capabilities in sodium cold traps used in nuclear reactor system loops.

Toluene can be inhaled for its intoxicating effects. Low to moderate levels can cause tiredness, confusion, weakness, drunken-type actions, memory loss, nausea, loss of appetite, and hearing and color vision loss. These symptoms usually disappear when exposure is stopped. Inhaling high levels of toluene in a short time may cause light-headedness, nausea, or sleepiness. It can also cause unconsciousness, and even death. Toluene may negatively affect kidney function.

Toluene has also been used in the process of removing the cocaine from coca leaves in the production of Coca-Cola syrup.
