GENERAL

1 4 di tert butyl 2 5 dimethoxybenzene msds

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Introduction

In the world of organic chemistry, the compound known as 1,4 di tert butyl 2,5 dimethoxybenzene is a fascinating molecule that combines steric bulk with electron donating methoxy groups. This unique structure lends itself to a range of applications, from advanced materials to fine chemical synthesis. However, as with any specialty reagent, safety is paramount. A comprehensive Material Safety Data Sheet (MSDS) – now commonly referred to as a Safety Data Sheet (SDS) – provides essential information for chemists, laboratory technicians, and industrial workers who handle the substance. This article delves into the chemical's properties, uses, synthesis, and most importantly, the safety considerations outlined in its MSDS.

What Is 1,4 Di tert butyl 2,5 Dimethoxybenzene?

The compound's systematic name, 1,4 di tert butyl 2,5 dimethoxybenzene, describes a benzene ring substituted with two bulky tert butyl groups at the para positions and two methoxy groups at the meta positions. The presence of tert butyl groups provides steric hindrance that can influence reactivity, while the methoxy groups act as strong electron donors, affecting the electron density of the aromatic ring. The molecular formula is C16H22O2, and the compound is typically a pale yellow liquid with a faint aromatic odor.

Key Physical and Chemical Properties

- Molecular weight: 226.33 g/mol
- Boiling point: ~260 /°C (decomposes)
- Melting point: –90 /°C (liquid at room temperature)
- Density: 0.88 g/mL at 20 /°C
- Solubility: Slightly soluble in water; highly soluble in organic solvents such as ethanol, acetone, and dichloromethane
- Flash point: 140 /°C (closed cup)

These properties highlight the compound's volatility and potential flammability, underscoring the importance of proper storage and handling protocols.

Applications and Industrial Relevance

While 1,4 di tert butyl 2,5 dimethoxybenzene may not be a household name, it plays a pivotal role in several high tech sectors:

1. Pharmaceutical intermediates: The molecule can serve as a building block for synthesizing complex drug candidates, especially those requiring sterically hindered aromatic cores.
2. Materials science: Its bulky substituents make it a useful precursor for polymerizable monomers that yield high performance plastics and resins.
3. Organic synthesis: The electron rich aromatic ring is an excellent substrate for electrophilic aromatic substitution reactions, enabling the introduction of diverse functional groups.
4. Research and development: Laboratories frequently employ the compound to study steric effects on reaction

mechanisms and to develop new catalytic processes.

Typical Synthetic Routes

Creating 1,4 di tert butyl 2,5 dimethoxybenzene often involves a multi step synthesis. A common approach starts with commercially available p tert butyl anisole. The process typically includes the following steps:

1. Selective methylation: The anisole is subjected to methylation using methyl iodide in the presence of a strong base, yielding a dimethoxy derivative.
2. Cross coupling: A palladium catalyzed cross coupling reaction introduces the second tert butyl group at the para position.
3. Purification: Flash chromatography or recrystallization removes side products, yielding the desired compound in high purity.

Alternative routes may employ directed ortho metalation or Friedel–Crafts alkylation, depending on the desired scale and available reagents.

Understanding the MSDS: An Overview

The Material Safety Data Sheet (MSDS), now standardized under the Globally Harmonized System (GHS) as a Safety Data Sheet (SDS), is a critical resource for anyone working with chemicals. It provides a snapshot of hazards, protective measures, first aid steps, and regulatory compliance information. For 1,4 di tert butyl 2,5 dimethoxybenzene, the MSDS contains the following key sections:

- Identification and recommended uses
- Hazard identification
- Composition and purity
- First aid measures
- Firefighting measures
- Accidental release measures
- Handling and storage
- Exposure controls and personal protection
- Physical and chemical properties
- Stability and reactivity
- Toxicological information
- Ecological information
- Disposal considerations
- Transport information
- Regulatory information
- Other relevant data

Reading and interpreting each section ensures safe usage and compliance with local and international regulations.

Hazard Identification and Classification

According to the GHS, 1,4 di tert butyl 2,5 dimethoxybenzene is classified as:

- Flammable liquid – Class 3
- Skin irritation – Category 2
- Eye irritation – Category 2
- Respiratory sensitization – Category 2

These classifications indicate that the compound can ignite easily, may cause skin and eye irritation, and could provoke allergic respiratory reactions in susceptible individuals. Appropriate safety measures, such as using a fume hood, wearing gloves and goggles, and avoiding inhalation, are essential.

Composition and Purity Details

The MSDS lists the compound’s purity as typically "e99%. Impurities, if present, are usually trace levels of solvents or by products from synthesis. Knowing the purity level is crucial for predicting reactivity and ensuring that analytical results are accurate. If the compound is used as a reagent, the SDS should also include the identity and concentration of any additives or stabilizers.

First Aid Measures

In case of accidental exposure, the SDS recommends the following:

- Inhalation: Move the person to fresh air immediately; if breathing is difficult, provide rescue breathing or oxygen.
- Skin contact: Wash affected area with plenty of soap and water for at least 15 minutes; remove contaminated clothing.
- Eye contact: Flush eyes with water for at least 15 minutes while keeping eyelids open; seek medical attention.
- Ingestion: Do not induce vomiting; seek immediate medical care.

These first aid steps are standard for many flammable, irritant chemicals, but always refer to the specific SDS for any compound specific guidance.

Firefighting Measures

Firefighters should use water spray, foam, or dry chemical extinguishers suitable for Class 3 flammable liquids. The SDS advises against using CO, or air driven extinguishers, as these can spread flammable vapors. Protective clothing, self contained breathing apparatus, and eye protection are recommended to protect firefighters from inhalation of toxic fumes and splashes.

Accidental Release Measures

Spills of 1,4 di tert butyl 2,5 dimethoxybenzene should be handled as follows:

1. Evacuate area: Ensure the area is free of ignition sources and that ventilation is adequate.
2. Contain spill: Use spill containment kits, absorbent pads, or inert absorbents (e.g., vermiculite).
3. Ventilate: Increase airflow to dissipate vapors.
4. Clean up: Wear appropriate PPE, collect spill material, and dispose of it according to local regulations.

These steps minimize the risk of fire, inhalation hazards, and environmental contamination.

Handling and Storage Guidelines

Safe handling involves:

- Using a well ventilated area or fume hood to prevent vapor accumulation.
- Wearing chemical resistant gloves (e.g., nitrile), safety goggles, and lab coats.
- Storing the compound in a tightly sealed, chemically compatible container (e.g., glass or high density polyethylene) in a cool, dry, well ventilated area away from oxidizers and heat sources.

- Labeling containers clearly with the chemical name, hazard pictograms, and SDS reference number.
- Keeping incompatible substances (e.g., strong acids, oxidizers) in separate compartments.

Exposure Controls and Personal Protective Equipment (PPE)

To limit occupational exposure, the SDS recommends:

- Engineering controls: Use of local exhaust ventilation or fume hoods.
- Administrative controls: Limit the duration of exposure and rotate tasks.
- Personal protective equipment: Chemical resistant gloves (nitrile), safety goggles, lab coat, and, if inhalation risk is high, a respirator rated for organic vapors.

Periodic monitoring of airborne concentrations (e.g., using personal sampling pumps) helps ensure that exposure remains below occupational exposure limits (OELs) established by agencies such as OSHA or ACGIH.

Physical and Chemical Properties Revisited

Reiterating the physical properties aids in quick reference:

- Appearance: Pale yellow liquid

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