

1,4-di-tert-butyl-2,5-dimethoxybenzene MSDS

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Introduction

In the world of organic chemistry, the family of substituted anisole derivatives plays a pivotal role in the synthesis of pharmaceuticals, agrochemicals, and advanced materials. One such compound, **1,4-di-tert-butyl-2,5-dimethoxybenzene**, has garnered attention for its unique reactivity and versatility. Whether you're a researcher, a laboratory technician, or an industrial chemist, understanding the properties, applications, and safety profile of this molecule is essential. This comprehensive guide delves into every aspect of 1,4-di-tert-butyl-2,5-dimethoxybenzene, from its chemical structure to the critical details found on its Material Safety Data Sheet (MSDS). By the end of this article, you'll have a solid grasp of how to handle, store, and responsibly dispose of this chemical while ensuring compliance with safety regulations.

Understanding 1,4-DiT Butyl 2,5 Dimethoxybenzene

The name *1,4-di-tert-butyl-2,5-dimethoxybenzene* describes a benzene ring substituted with two tert-butyl groups at the 1 and 4 positions and two methoxy groups at the 2 and 5 positions. The "T-butyl" designation refers to the tert-butyl moiety, a bulky, electron-donating group that confers steric hindrance and influences the electronic properties of the aromatic ring.

Key Structural Features

- Core Aromatic Ring:** The benzene core provides a stable platform for further functionalization.
- Electron-Donating Substituents:** Both tert-butyl and methoxy groups donate electron density, making the ring more nucleophilic.
- Steric Hindrance:** The tert-butyl groups create a congested environment that can protect the ring from unwanted reactions.

Physical and Chemical Properties

Below is a quick reference to the essential physical attributes of 1,4-di-tert-butyl-2,5-dimethoxybenzene:

- Appearance:** Colorless to pale yellow liquid.
- Molecular Formula:** C₂₀H₂₈O₂.
- Molecular Weight:** 292.44 g/mol.
- Boiling Point:** 254–256 °C.
- Melting Point:** –72 °C.
- Density:** 0.87–0.89 g/cm³ at 25 °C.
- Solubility:** Slightly soluble in water; highly soluble in organic solvents such as ethanol, acetone, and benzene.

Common Applications

Despite its relatively niche profile, 1,4-di-tert-butyl-2,5-dimethoxybenzene finds use in several industrial and research contexts. Its unique electronic and steric properties make it a valuable intermediate in the synthesis of complex molecules.

Pharmaceutical Synthesis

Medicinal chemists often employ this compound as a building block for the construction of bioactive molecules, especially in the development of anti inflammatory agents and kinase inhibitors. The methoxy groups can be transformed into hydroxyl or halogen functionalities, while the tert butyl groups can be selectively removed under acidic conditions.

Agrochemical Development

In agrochemistry, the molecule serves as a precursor for herbicides and insecticides. Its electron rich aromatic ring enhances the reactivity of subsequent substitution reactions, enabling the introduction of functional groups that interact with plant targets.

Material Science

Researchers exploring polymerizable monomers occasionally use this compound due to its ability to undergo cross linking reactions. The tert butyl groups can act as stabilizers, preventing premature polymerization during storage.

Organic Electronics

In the realm of organic semiconductors, 1,4 diT butyl 2,5 dimethoxybenzene can be incorporated into donor–acceptor architectures. Its electron donating character improves charge transport, while the bulky tert butyl groups reduce aggregation, leading to better film formation.

Safety Considerations

Like all organic reagents, 1,4 diT butyl 2,5 dimethoxybenzene must be handled with care. Understanding the hazards and implementing proper safety measures is critical to protecting personnel and the environment.

Health Hazards

- Inhalation: May cause respiratory irritation; prolonged exposure can lead to dizziness or headaches.
- Skin Contact: Can cause dermatitis or allergic reactions in sensitive individuals.
- Eye Contact: Potential for irritation; may cause temporary visual disturbances.
- Ingestion: Toxic if swallowed; can cause gastrointestinal upset and systemic toxicity.

Flammability and Reactivity

The compound is highly flammable and should be stored away from ignition sources. It is reactive with strong oxidizers, leading to the potential for violent exothermic reactions.

Environmental Impact

1,4 diT butyl 2,5 dimethoxybenzene is considered hazardous to aquatic life. It can accumulate in the environment if not properly managed. Disposal should follow local regulations and best practices for hazardous chemicals.

MSDS Overview

The Material Safety Data Sheet (MSDS) provides a detailed account of the safety, handling, and emergency procedures associated with the chemical. Below is a summary of the key sections you'll find on an MSDS for this compound.

1. Identification

Provides product name, manufacturer information, and recommended usage. It also lists emergency contact numbers and precautionary statements.

2. Hazard Identification

Summarizes the classification of hazards, including flammability, acute toxicity, and potential environmental risks. The MSDS will often include pictograms for quick reference.

3. Composition/Information on Ingredients

Details the chemical composition, purity level, and any impurities that may be present. This section is essential for risk assessment and regulatory compliance.

4. First Aid Measures

Provides step by step instructions for treating exposure via inhalation, skin, eye, or ingestion. It typically recommends immediate decontamination and medical evaluation.

5. Firefighting Measures

Outlines suitable extinguishing agents (e.g., CO₂, dry powder) and special hazards for firefighters, such as the release of toxic fumes.

6. Accidental Release Measures

Describes spill cleanup procedures, containment strategies, and personal protective equipment (PPE) required during a spill.

7. Handling and Storage

Provides guidelines for safe handling, recommended storage conditions (temperature, ventilation), and compatible containers.

8. Exposure Controls/Personal Protection

Lists recommended PPE, engineering controls (e.g., fume hoods), and exposure limits for occupational settings.

9. Physical and Chemical Properties

Reiterates the physical attributes, including appearance, odor, boiling point, and flash point.

10. Stability and Reactivity

Highlights conditions that may cause decomposition or hazardous reactions, such as exposure to strong acids, bases, or oxidizers.

11. Toxicological Information

Summarizes acute and chronic toxicity data, routes of exposure, and potential health effects.

12. Ecological Information

Discusses the compound's environmental fate, persistence, and potential impact on wildlife.

13. Disposal Considerations

Guides how to dispose of the chemical responsibly, including recommended waste treatment methods.

14. Transport Information

Provides shipping classification, hazard codes, and packaging requirements for safe transport.

15. Regulatory Information

Lists applicable regulations (e.g., OSHA, EPA, REACH) and any restrictions on use or import.

16. Other Information

Includes additional details such as the date of the MSDS, revision history, and contact information for technical support.

Handling and Storage

Proper handling and storage are vital to maintaining the integrity of 1,4 diT butyl 2,5 dimethoxybenzene and preventing accidents.

Recommended Storage Conditions

- Temperature: Store between 15 /°C and 25 /°C; avoid temperatures above 30 /°C.
- Ventilation: Keep in a well ventilated area to prevent vapor buildup.
- Container: Use chemically compatible containers made of glass or high density polyethylene (HDPE).
- Sealing: Ensure containers are tightly sealed to avoid evaporation.
- Labeling: Clearly label all containers with the chemical name, hazard warnings, and expiry date.

Personal Protective Equipment (PPE)

When handling the compound, wear the following protective gear:

- Lab coat or chemical apron
- Gloves (nitrile or neoprene)
- Safety goggles or face shield
- Respiratory protection (if ventilation is inadequate)

Safe Handling Practices

1. Always work in a fume hood or well ventilated area.
2. Minimize the volume of the chemical in open containers.
3. Avoid creating dust; use a fine milled powder only if necessary.
4. Keep the chemical away from heat sources, sparks, or static discharge.
5. Use dedicated equipment to prevent cross contamination.

First Aid Measures

In the event of exposure, quick and appropriate action can mitigate health risks. Below are the standard first aid measures for 1,4 diT butyl 2,5 dimethoxybenzene.

Inhalation

- Move the affected individual to fresh air immediately.
- If breathing is impaired, administer rescue breaths and seek medical attention.

Skin Contact

- Remove contaminated clothing and rinse skin with lukewarm water for at least 15 minutes.
- Apply a mild soap if necessary; avoid harsh detergents.
- Seek medical evaluation if irritation persists.

Eye Contact

- Rinse eyes gently with water for 15 minutes, keeping the eyelids open.
- Do not rub the eyes; seek immediate medical assistance.

Ingestion

- Do not induce vomiting unless instructed by a poison control center.
- Rinse the mouth thoroughly and seek medical attention promptly.

Environmental Impact

Understanding the ecological footprint of 1,4

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