Product Safety Summary

4-tert-Octylphenol

This product safety summary is intended to provide a general overview of the chemical substance. The information on the Summary is basic information and is not intended to provide emergency response information or information on medical treatment. Additional information on this substance is available on its Material Safety Data Sheet which should be consulted prior to using the chemical.

1) Chemical Identity

Name: 4-tert-Octylphenol
Abbreviation: PTOP
Common Names: Phenol, 4-(1,1,3,3-tetramethylbutyl)-;
4-tertiary-Octylphenol; para-tert-Octylphenol
CAS Number: 140-66-9
EINECS Number: 205-426-2

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\begin{align*}
\text{HO} & \quad \text{CH}_3 \\
\text{C-CH}_2 & \quad \text{C-CH}_3 \\
\text{CH}_3 & \quad \text{CH}_3
\end{align*}
\]

2) Product Overview

4-tert-Octylphenol has the chemical formula C_{14}H_{22}O. It is a white to pale yellow crystalline solid at room temperature and is sold in solid form as flakes or briquettes in 25 kg bags or in super sacks of either 350 or 500 kg. PTOP may also be sold in molten form in tank trucks or rail cars. In this form, the product must be heated to 200-210°F (90-100°C) to assure that it is completely molten prior to off-loading into storage facilities via pipeline. In molten form, PTOP can cause thermal burns due to its elevated temperature.

PTOP is a chemical intermediate which is exclusively marketed to other professional chemical companies for the purpose of acting as an intermediate raw material to be transformed into other chemical products. PTOP has no direct applications in its own right and is not intended as a direct component of any consumer product.

3) The Main End Uses For PTOP Include:

- As a monomer for alkylphenol formaldehyde resins used in rubber, coatings, insulating varnishes, printing inks, etc.
- As a chain initiation intermediate for the production of alkylphenol ethoxylates used in nonionic surfactants, emulsion polymerization and as a general emulsifying agent.
- As a chain terminating agent in the production of polycarbonate plastics.
- As an intermediate for organic synthesis.
4) Physical Properties

- Physical state / appearance at 77ºF (25°C) white to pale yellow flakes
- Odour: weak phenolic
- Density: 0,940 g/cm³ @ 77ºF (25°C)
- Solubility in water (bulk): 7 mg/L @ 68ºF (20°C)
- Vapor pressure: 0,02 mbar @ 100ºF (38°C)
- Melting point: 185ºF (85°C)
- Boiling point: 372ºF (189ºC) @ 101 kPa
- Flash point (Tag closed cup): 269ºF (132°C)
- Self ignition temperature: 680ºF (360°C)
- Log Kow: 4,8 @ 72ºF (22°C)

5) Health Information

Octylphenol caused the following effects in animal studies. The relevance of these findings to humans is not known.

PTOP is:
- A low concern for acute toxicity by the oral or dermal route of exposure; signs of toxicity and mortality occur at very high dose levels that are much greater than typical human exposure
- Irritating to skin and may cause eye damage
- Not a skin sensitizer
- Not mutagenic or clastogenic
- A low concern for carcinogenicity by genotoxic and non-genotoxic mechanisms
- The results of the two-generation study indicate that PTOP is not toxic to reproduction in mammals over a wide range of doses (Tyl, R.W. et al (1999), Reg. Toxicol. Pharmacol., 30, 81-95)

<table>
<thead>
<tr>
<th>Species</th>
<th>End Point</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rabbit</td>
<td>Acute Dermal Exposure</td>
<td>LD50 = &gt;2000 mg/kg</td>
</tr>
<tr>
<td>Rat</td>
<td>Acute Oral Toxicity</td>
<td>LD50 = 4040 mg/kg</td>
</tr>
<tr>
<td>Rabbit</td>
<td>Eye Irritation</td>
<td>severe</td>
</tr>
<tr>
<td>Rabbit</td>
<td>Skin Irritation</td>
<td>mild</td>
</tr>
</tbody>
</table>

6) Environmental Effects

4-tert-Octylphenol is very toxic to aquatic organisms. Special care should be taken to assure that PTOP or mixtures containing PTOP do not enter the aquatic environment.

<table>
<thead>
<tr>
<th>Species</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fish (Rainbow trout), 96-hr</td>
<td>LC50 = &gt;0,1 mg/L</td>
</tr>
<tr>
<td>Daphnia magna, 96-hr</td>
<td>EC50 = 0,0133 mg/L</td>
</tr>
<tr>
<td>Algae, 96-hr</td>
<td>EC50 = 1,9 mg/L</td>
</tr>
</tbody>
</table>
Environmental Fate

PTOP is inherently biodegradable. The bioconcentration fact (BCF) is 740 L/kg not indicating an elevated bioaccumulation potential. It is photolytically degradable. In the atmospheric compartment its half-life is estimated at 6 hours.

7) Exposure Potential

Manufacturing

The manufacture of PTOP is conducted in a continuous process via the catalyzed reaction of phenol and diisobutylene. After recycle streams are taken into account, all reactants are essentially 100% utilized and converted to product. The chemical reactions are carried out in closed reactors under strictly controlled conditions aided by modern process control computers. Raw materials are added by dedicated pipelines so that there is no worker exposure or environmental release during the process. Chemical operators oversee the reaction conditions in the manufacturing plants. These individuals are highly trained in chemical processing and handling as well as in the correct use of safety equipment and engineering controls. It is customary for chemical operators to use personal protection equipment that includes coveralls, long sleeve shirts, work shoes with protective coverings, eye and face protection, chemical resistant gloves and hardhats.

Finished products are isolated by distillation and are handled in a closed system of pipes and dedicated storage tanks. There is no opportunity for dermal or inhalation exposure during the product transfer process.

Reaction products are monitored for quality assurance (QA) using aliquots of the vessel contents collected from controlled sampling spigots that precludes aerosol formation, splashing or spillage due to overflow. Samples analyzed in the QA lab are handled using good laboratory safety practices. No exposure to PTOP is expected during the sampling or analytical processes.

Maintenance worker exposure to PTOP during cleaning operations for storage vessels or shipping tanks is eliminated when proper engineering controls and required personal protective equipment are in use. Railcars and tank trucks are typically steam cleaned in an automated fashion. Workers complete the cleaning of these enclosures while wearing suitable personal protective equipment that includes chemical suits and respirators designed to protect against exposure.

Flaked Or Packaged Products

The generation of flake or briquetted PTOP involves the application of a uniform, thin film of molten product to a cold surface from which the solidified material is recovered for further processing and packaging. Exposure to vapor or dust from manufacturing operations is accomplished via engineering controls in the production area. Dermal or inhalation exposure to dust or solid PTOP from packaged material by downstream users should be avoided.

Accumulated dust from the use of PTOP in solid form (or any other combustible dust) represents a potential explosion hazard. Special care should be taken to avoid the accumulation of dust in any work areas using good industrial hygiene practices.
Consult the relevant Material Safety Data Sheet for specific handling and packaging disposal precautions.

**Consumer Products**

PTOP has no direct application in consumer products and is only sold to professional chemical companies for use as a chemical intermediate which is transformed into other substances.

**8) Risk Management Recommendations**

Good general ventilation (typically 10 air changes per hour) should be used. Ventilation rates should be matched to conditions. If applicable, use process enclosures, local exhaust ventilation, or other engineering controls to maintain airborne levels below recommended exposure limits. If exposure limits have not been established, maintain airborne levels to an acceptable level. Ventilation should be sufficient to effectively remove, and prevent buildup of, any vapors, dusts, or fumes that may be generated during handling or thermal processing. In order to ensure appropriate electrical safety practices are followed, consult applicable standards. These may include guidelines such as the National Fire Protection Association [NFPA] 70, "The National Electrical Code" and NFPA 499, "Recommended Practice for the Classification of Combustible Dusts and of Hazardous (Classified) Locations for Electrical Installations in Chemical Process Areas ". NOTE: since this material's vapors, dust or fumes can form explosive mixtures in air, ensure that any potential areas where explosions may occur are designed to minimize potential damage. For recommendations to prevent such explosions and associated damage, consult applicable guidelines such as NFPA 69, "Standard on Explosion Prevention Systems" and/or NFPA 68, "Guide for Venting Deflagrations". Keep working clothes separately and do not take them home

**9) State Agency Review**

4-tert-Octylphenol has been registered under REACH Regulation (EC) 1907/2006. A SIDS Initial Assessment Report and Environmental Risk Evaluation Report are available.


**10) Regulatory Information, Classification and Labelling**

GHS classification of PTOP according CLP (CE) 1272/2008:

- Skin corrosion/irritation  Category 2 H315 Causes skin irritation
- Serious eye damage/eye irritation  Category 1 H318 Causes serious eye damage
- Hazardous to the aquatic Environment, long-term hazard  Category 1 H410 Very toxic to aquatic life with long lasting effects

Signal Word: Danger
11) Conclusion

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12) Contact Information within Company

For further information please contact: sds.info@siigroup.com