**IDENTIFICATION**

**MSDS Record Number:** 5618711  
**Product Name(s):** 2,2,4-TRIMETHYLPENTANE  
**Product Identification:**  
- PRODUCT CODE: 9335, 9478, 9479, 9480, W898, 1943, 5633, 6043, 6051, 6052, V559  
- C.A.S. NUMBER: 540-84-1  
**Date of MSDS:** 2007-05-04  
**Currency Note:** This MSDS was acquired from the supplier on 2007-09-06.

**MANUFACTURER/SUPPLIER INFORMATION**

**Company:** MALLINCKRODT BAKER INC

**MATERIAL SAFETY DATA**

**Effective Date:** 05/04/07  
**Supersedes:** 08/10/04

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**MSDS MATERIAL SAFETY DATA SHEET**

From: Mallinckrodt Baker, Inc.  
222 Red School Lane  
Phillipsburg, NJ 08865  

Emergency Telephone Number: 908-859-2151  

NOTE: Use CHEMTREC and CANUTEC phone numbers only in the event of a chemical emergency.

All non-emergency questions should be directed to Customer Service (1-800-582-2537) for assistance.

M A L L I N C R O D T  J. T. B A K E R

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**2,2,4-TRIMETHYLPENTANE**

1. **Product Identification**

- **Synonyms:** iso-octane; isobutytrimethylmethane  
- **CAS No:** 540-84-1  
- **Molecular Weight:** 114.23  
- **Chemical Formula:** (CH3)3C(CH2CH(CH3)2
- **Product Codes:** J.T. Baker:  
  - 9335, 9478, 9479, 9480, W898  
  - Mallinckrodt:
1943, 5633, 6043, 6051, 6052, V559

2. Composition/Information on Ingredients

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>CAS No</th>
<th>Percent</th>
<th>Hazardous</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pentane, 2,2,4-trimethyl-</td>
<td>540-84-1</td>
<td>99 - 100%</td>
<td>Yes</td>
</tr>
</tbody>
</table>

3. Hazards Identification

Emergency Overview

DANGER! EXTREMELY FLAMMABLE LIQUID AND VAPOR. VAPOR MAY CAUSE FLASH FIRE. HARMFUL OR FATAL IF SWALLOWED. HARMFUL IF INHALED. CAUSES IRRITATION TO SKIN, EYES AND RESPIRATORY TRACT. AFFECTS CENTRAL NERVOUS SYSTEM. SAF-T-DATA(tm) Ratings (Provided here for your convenience)

Health Rating: 2 - Moderate
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:
May cause symptoms similar to those of ingestion. High concentrations may cause dizziness, lack of coordination, and narcosis. Concentrations of about 16,000 ppm may cause respiratory arrest.

Ingestion:
May cause nausea, vomiting, pulmonary irritation, edema, bloody sputum, and bronchial pneumonia with fever and coughing when aspirated. If large doses (> 1ml/kg) are ingested and retained symptoms of central nervous system depression may occur and include shallow respiration, unconsciousness, and convulsions. May cause ventricular fibrillation, kidney, liver and bone marrow damage.

Skin Contact:
Causes skin irritation. May cause an allergic dermatitis.

Eye Contact:
Causes irritation; symptoms including redness, itching, and pain.

Chronic Exposure:
Prolonged or repeated skin contact may cause dermatitis.

Aggravation of Pre-existing Conditions:
Persons with pre-existing skin disorders or impaired pulmonary function may be more susceptible to the effects of this substance.

4. First Aid Measures

Inhalation:
Remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Call a physician.

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.

Skin Contact:
Remove any contaminated clothing. Wash skin with soap or mild detergent and water for at least 15 minutes. Wash clothes before reuse. Get medical attention if irritation develops or persists.

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

5. Fire Fighting Measures
Fire:
Flash point: -12C (10F) CC
Autoignition temperature: 415C (779F)
Flammable limits in air % by volume:
lel: 1.1; uel: 6.0
Extremely Flammable Liquid and Vapor! Vapor may cause flash fire.
Explosion:
Above flash point, vapor-air mixtures are explosive within flammable limits noted above. Vapors can flow along surfaces to distant ignition source and flash back. Sealed containers may rupture when heated. Contact with strong oxidizers may cause fire. Sensivel a descargas estáticas.
Fire Extinguishing Media:
Dry chemical, foam or carbon dioxide. Water may be ineffective. Water spray may be used to keep fire exposed containers cool.
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. This highly flammable liquid must be kept from sparks, open flame, hot surfaces, and all sources of heat and ignition.

6. 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! Have foam or dry powder extinguisher on hand. Small spills will evaporate. 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.
J. T. Baker SOLUSORB(R) solvent adsorbent is recommended for spills of this product.

7. 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. Do Not attempt to clean empty containers since residue is difficult to remove. Do not pressurize, cut, weld, braze, solder, drill, grind or expose such containers to heat, sparks, flame, static electricity or other sources of ignition: they may explode and cause injury or death.

8. Exposure Controls/Personal Protection
Airborne Exposure Limits:
-OSHA Permissible Exposure Limit (PEL): 500 ppm (TWA) for (Petroleum

Distillates)
-NIOSH (REL): 10Hr.TWA, 350mg/m³, 1800 mg/m³ 15min. Ceiling for (Refined Petroleum Distillates)
-ACGIH Threshold Limit Value (TLV): 300 ppm (TWA) for (iso-octane).

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):
For conditions of use where exposure to the substance is apparent and engineering controls are not feasible, consult an industrial hygienist. For emergencies, or instances where the exposure levels are not known, use a full-facepiece 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. Maintain eye wash fountain and quick-drench facilities in work area.

9. Physical and Chemical Properties

Boiling Point:
99°C (210°F)

Melting Point:
-107°C (-161°F)

Vapor Density (Air=1):
3.9

Vapor Pressure (mm Hg):
ca. 41 @ 21°C (70°F)

Evaporation Rate (BuAc=1):
< 1 (Ether = 1)

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

10. Stability and Reactivity

Stability:
Stable under ordinary conditions of use and storage.

Hazardous Decomposition Products:
Carbon dioxide and carbon monoxide may form when heated to decomposition.

Hazardous Polymerization:
Will not occur.

Incompatibilities:
Strong oxidizing agents, strong reducing agents, strong acids or bases.

Conditions to Avoid:
Heat, flames, ignition sources and incompatibles.

11. Toxicological Information
No LD₅₀/LC₅₀ information found relating to normal routes of occupational exposure. Investigated as a mutagen.

---NTP Carcinogen---

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>Known</th>
<th>Anticipated</th>
<th>IARC Category</th>
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<tbody>
<tr>
<td>Pentane, 2,2,4-trimethyl-</td>
<td>No</td>
<td>No</td>
<td>None</td>
</tr>
</tbody>
</table>

12. Ecological Information
Environmental Fate:
When released into the soil, this material may biodegrade to a moderate extent. When released into the soil, this material is not expected to leach into groundwater. When released into the soil, this material is expected to quickly evaporate. When released into water, this material may biodegrade to a moderate extent. When released to water, this material is expected to quickly evaporate. When released into the water, this material is expected to have a half-life of less than 1 day. This material may bioaccumulate to some extent. When released into the air, this material is expected to be readily degraded by reaction with photochemically produced hydroxyl radicals. When released into the air, this material is not expected to be degraded by photolysis. When released into the air, this material is expected to have a half-life between 1 and 10 days.

Environmental Toxicity:
No information found.

13. Disposal Considerations
Whatever cannot be saved for recovery or recycling should be handled as hazardous waste and sent to a RCRA approved incinerator or disposed in a RCRA approved waste facility. Processing, use or contamination of this product may change the waste management options. State and local disposal regulations may differ from federal disposal regulations.
Dispose of container and unused contents in accordance with federal, state and local requirements.

14. Transport Information
Domestic (Land, D.O.T.)

Proper Shipping Name: OCTANES
Hazard Class: 3
UN/NA: UN1262 Packing Group: II
Information reported for product/size: 313LB

International (Water, I.M.O.)

Proper Shipping Name: OCTANES
Hazard Class: 3
UN/NA: UN1262 Packing Group: II
Information reported for product/size: 313LB

15. Regulatory Information

\Chemical Inventory Status - Part 1\-

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<th>Ingredient</th>
<th>TSCA</th>
<th>EC</th>
<th>Japan</th>
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<tbody>
<tr>
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<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
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\Chemical Inventory Status - Part 2\-

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<th>Ingredient</th>
<th>Korea</th>
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<td>Yes</td>
<td>Yes</td>
<td>No</td>
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</table>

\Federal, State & International Regulations - Part 1\-

- SARA 302 - SARA 313 -

<table>
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<th>Ingredient</th>
<th>RQ</th>
<th>TPQ</th>
<th>List</th>
<th>Chemical Ctg.</th>
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</table>

| Pentane, 2,2,4-trimethyl- (540-84-1) | No | No | No | No |

\Federal, State & International Regulations - Part 2\-
<table>
<thead>
<tr>
<th>Ingredient</th>
<th>CERCLA</th>
<th>RCRA</th>
<th>TSCA</th>
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<tr>
<td>Pentane, 2,2,4-trimethyl- (540-84-1)</td>
<td>1000</td>
<td>No</td>
<td>No</td>
</tr>
</tbody>
</table>

Chemical Weapons Convention: No  
TSCA 12(b): No  
CDTA: No  
SARA 311/312: Acute: Yes Chronic: No  
Fire: Yes Pressure: No  
Reactivity: No  
(Pure / Liquid)

Australian Hazchem Code: 3[Y]E  
Australian Poison Schedule: None allocated.

WHMIS:  
This MSDS has been prepared according to the hazard criteria of the Controlled Products Regulations (CPR) and the MSDS contains all of the information required by the CPR.

16. Other Information

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

Label Hazard Warning:
DANGER! EXTREMELY FLAMMABLE LIQUID AND VAPOR. VAPOR MAY CAUSE FLASH FIRE. HARMFUL OR FATAL IF SWALLOWED. HARMFUL IF INHALED. CAUSES IRRITATION TO SKIN, EYES AND RESPIRATORY TRACT. AFFECTS CENTRAL NERVOUS SYSTEM.

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

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 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. In all cases call a physician.

Product Use:
Laboratory Reagent.

Revision Information:
No Changes.

Disclaimer:
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T6526
