



# MATERIAL SAFETY DATA SHEET

according to the Global Harmonized System

Date of issue: 02/04/2013

Version 1.0

## SECTION 1. Identification

### Product identifier

Product number 814693  
Product name (2-tert-Butyl-4-methylcyclohexyl) acetate (mixture of isomers) for synthesis

### Relevant identified uses of the substance or mixture and uses advised against

Identified uses Chemical for synthesis

### Details of the supplier of the safety data sheet

Company EMD Millipore Corporation | 290 Concord Road, Billerica, MA 01821, United States of America | SDS Phone Support: +1-978-715-1335 | General Inquiries: +1-978-751-4321 | Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)  
e-mail: mm\_sds@merckgroup.com

Emergency telephone 613-996-6666 CANUTEC (Canada)  
+1-703-527-3887 CHEMTREC (International)  
24 Hours/day; 7 Days/week

## SECTION 2. Hazards identification

### GHS-Labeling

Not a hazardous substance or mixture according to Regulation (EC) No 1272/2008.

### Other hazards

None known.

## SECTION 3. Composition/information on ingredients

Chemical nature Mixture of isomers.  
Formula  $C_{13}H_{24}O_2$  (Hill)  
CAS-No. 115724-27-1  
Molar mass 212.34 g/mol

Remarks WHMIS hazardous composition: No ingredients are hazardous according to the CPR criteria.

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#### SECTION 4. First aid measures

##### Description of first-aid measures

###### *Inhalation*

After inhalation: fresh air. Consult doctor if feeling unwell.

###### *Skin contact*

After skin contact: wash off with plenty of water. Remove contaminated clothing.

###### *Eye contact*

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist.

###### *Ingestion*

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Never give anything by mouth to an unconscious person.

##### Most important symptoms and effects, both acute and delayed

We have no description of any toxic symptoms.

##### Indication of any immediate medical attention and special treatment needed

No information available.

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#### SECTION 5. Fire-fighting measures

##### Extinguishing media

###### *Suitable extinguishing media*

Carbon dioxide (CO<sub>2</sub>), Foam, Dry powder

###### *Unsuitable extinguishing media*

For this substance/mixture no limitations of extinguishing agents are given.

##### Special hazards arising from the substance or mixture

Combustible material, Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapors possible in the event of fire.

Forms explosive mixtures with air on intense heating.

##### Advice for firefighters

###### *Special protective equipment for fire-fighters*

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

###### *Further information*

Prevent fire extinguishing water from contaminating surface water or the ground water system.

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#### SECTION 6. Accidental release measures

##### Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Do not breathe vapors, aerosols.

Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

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**Environmental precautions**

Do not empty into drains.

**Methods and materials for containment and cleaning up**

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7 and 10).

Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

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**SECTION 7. Handling and storage**

**Precautions for safe handling**

Observe label precautions.

**Conditions for safe storage, including any incompatibilities**

Tightly closed.

Store at +15°C to +25°C (+59°F to +77°F).

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**SECTION 8. Exposure controls/personal protection**

**Exposure limit(s)**

Contains no substances with occupational exposure limit values.

**Engineering measures**

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

**Individual protection measures**

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

*Hygiene measures*

Change contaminated clothing. Application of skin- protective barrier cream recommended.  
Wash hands after working with substance.

*Eye/face protection*

Safety glasses

*Hand protection*

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

*Respiratory protection*

required when vapors/aerosols are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

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**SECTION 9. Physical and chemical properties**

Physical state liquid

Color colorless

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Odor	pleasant
Odor Threshold	No information available.
pH	7.5 at 100 g/l 68 °F (20 °C) (as an emulsion)
Solidification point	15.2 °C
Boiling point/boiling range	140 - 158 °F (60 - 70 °C) at 0.4 hPa
Flash point	205 °F (96 °C) DIN 51758
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapor pressure	< 1 hPa at 122 °F (50 °C)
Relative vapor density	No information available.
Relative density	0.925 g/cm <sup>3</sup> at 77 °F (25 °C)
Water solubility	at 68 °F (20 °C) insoluble
Partition coefficient: n-octanol/water	No information available.
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	No information available.
Ignition temperature	509 °F (265 °C) DIN 51794

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**SECTION 10. Stability and reactivity**

**Reactivity**

Forms explosive mixtures with air on intense heating.

**Chemical stability**

The product is chemically stable under standard ambient conditions (room temperature) .

**Possibility of hazardous reactions**

Violent reactions possible with:

Strong oxidizing agents

**Conditions to avoid**

Strong heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

**Incompatible materials**

no information available

**Hazardous decomposition products**

no information available

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**SECTION 11. Toxicological information**

**Information on toxicological effects**

*Likely route of exposure*

Eye contact, Skin contact

*Acute oral toxicity*

LD50 rat: > 5,000 mg/kg (External MSDS)

*Acute dermal toxicity*

LD50 rat: > 2,000 mg/kg  
(External MSDS)

*Skin irritation*

rabbit

Result: No irritation  
(External MSDS)

*Eye irritation*

rabbit

Result: No eye irritation  
(External MSDS)

*Sensitization*

Sensitization test: guinea pig  
Result: negative  
(External MSDS)

*Specific target organ systemic toxicity - single exposure*

The substance or mixture is not classified as specific target organ toxicant, single exposure.

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*Specific target organ systemic toxicity - repeated exposure*

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

*Aspiration hazard*

Regarding the available data the classification criteria are not fulfilled.

**Carcinogenicity**

IARC	No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
NTP	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
ACGIH	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

**Further information**

Hazardous properties cannot be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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**SECTION 12. Ecological information**

**Ecotoxicity**

No information available.

**Persistence and degradability**

No information available.

**Bioaccumulative potential**

No information available.

**Mobility in soil**

No information available.

**Other adverse effects**

*Additional ecological information*

We have no quantitative data concerning the ecological effects of this product.

Further information on ecology

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**SECTION 13. Disposal considerations**

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

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**SECTION 14. Transport information**

**Land transport (DOT)**

Not classified as dangerous in the meaning of transport regulations.

**Air transport (IATA)**

Not classified as dangerous in the meaning of transport regulations.

**Sea transport (IMDG)**

Not classified as dangerous in the meaning of transport regulations.

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**SECTION 15. Regulatory information**

**United States of America**

**Canada**

**WHMIS Classification**

Not controlled under WHMIS (Canada).

This product has been classified according to the hazard criteria of the CPR and the MSDS contains all of the information required by the CPR.

**Notification status**

TSCA: On TSCA Inventory

DSL: This product contains one or several components listed in the Canadian NDSL.  
*Ingredients*  
2-(1,1-dimethylethyl)-4-methyl-cyclohexanol acetate

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**SECTION 16. Other information**

**Training advice**

Provide adequate information, instruction and training for operators.

**Key or legend to abbreviations and acronyms used in the safety data sheet**

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

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The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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