



# MATERIAL SAFETY DATA SHEET

according to the Hazard Communication Standard (29 CFR 1910.1200)

Revision Date 12/12/2012

Version 1.3

## SECTION 1. Identification

### Product identifier

Product number 845134  
Product name 4-Carboxybutyltriphenylphosphonium bromide for pharma synthesis, non-GMP

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

Identified uses Use restricted under TSCA to research and development or as analytical reagent. Uses regulated under FDA or FIFRA are not affected.  
Pharmaceutical production, 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 800-424-9300 CHEMTREC (USA)  
+1-703-527-3887 CHEMTREC (International)  
24 Hours/day; 7 Days/week

## SECTION 2. Hazards identification

### GHS-Labeling

*Precautionary Statements*  
P260 Do not breathe dust.  
P280 Wear protective gloves.

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

### OSHA Hazards

This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

### Other hazards

None known.

## SECTION 3. Composition/information on ingredients

Formula  $(C_6H_5)_3P(CH_2)_4COOH \cdot Br$   $C_{23}H_{24}BrO_2P$  (Hill)

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CAS-No. 17814-85-6

Molar mass 443.31 g/mol

Remarks No hazardous ingredients according to the OSHA Hazard Communication Standard 29 CFR 1910.1200.

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## SECTION 4. First aid measures

### Description of first-aid measures

#### *Inhalation*

After inhalation: fresh air.

#### *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.

#### *Ingestion*

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

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*

Water, 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.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

Fire may cause evolution of:

hydrogen bromide, Oxides of phosphorus

### 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*

Suppress (knock down) gases/vapors/mists with a water spray jet. 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 inhalation of dusts. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

#### 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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

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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. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

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. 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 dusts 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	powder
Color	white
Odor	weak
Odor Threshold	No information available.
pH	No information available.
Melting point	399 - 406 °F ( 204 - 208 °C)
Boiling point	No information available.
Flash point	383 °F ( 195 °C)
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	No information available.
Relative vapor density	No information available.
Relative density	No information available.
Water solubility	at 68 °F ( 20 °C) soluble
Partition coefficient: n-octanol/water	log Pow: 0.15 (calculated) (Lit.) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Bulk density	360 - 400 kg/m <sup>3</sup>

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**SECTION 10. Stability and reactivity**

**Reactivity**

Forms explosive mixtures with air on intense heating.  
The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

**Chemical stability**

sensitive to moisture

**Possibility of hazardous reactions**

Violent reactions possible with:  
Bases, bases, Amines, Ammonia

**Conditions to avoid**

Strong heating.

**Incompatible materials**

no information available

**Hazardous decomposition products**

in the event of fire: See section 5.

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**SECTION 11. Toxicological information**

**Information on toxicological effects**

*Likely route of exposure*

Inhalation, Eye contact, Skin contact, Ingestion

*Specific target organ systemic toxicity - single exposure*

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

*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.

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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

Quantitative data on the toxicity of this product are not available.

Further toxicological data:

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Further data:

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

*Partition coefficient: n-octanol/water*

log Pow: 0.15

(calculated)

(Lit.) Bioaccumulation is not expected (log Pow <1).

### Mobility in soil

No information available.

### Other adverse effects

*Additional ecological information*

Discharge into the environment must be avoided.

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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)

**UN number** UN 3464  
**Proper shipping name** ORGANOPHOSPHORUS COMPOUND, TOXIC, SOLID, N.O.S. ( 4-CARBOXYBUTYL-TRIPHENYL-PHOSPHONIUMBROMIDE)  
**Class** 6.1  
**Packing group** II  
**Environmentally hazardous** --

### Air transport (IATA)

**UN number** UN 3464  
**Proper shipping name** ORGANOPHOSPHORUS COMPOUND, TOXIC, SOLID, N.O.S. ( 4-CARBOXYBUTYL-TRIPHENYL-PHOSPHONIUMBROMIDE)  
**Class** 6.1  
**Packing group** II  
**Environmentally hazardous** --  
**Special precautions for user** no

### Sea transport (IMDG)

**UN number** UN 3464  
**Proper shipping name** ORGANOPHOSPHORUS COMPOUND, TOXIC, SOLID, N.O.S. ( 4-CARBOXYBUTYL-TRIPHENYL-PHOSPHONIUMBROMIDE)  
**Class** 6.1  
**Packing group** II  
**Environmentally hazardous** --  
**Special precautions for user** yes  
**EmS** F-A S-A

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## SECTION 15. Regulatory information

### United States of America

#### OSHA Hazards

Combustible dust

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

#### SARA 311/312 Hazards

No SARA Hazards

#### Clean Water Act

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This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

### US State Regulations

#### Massachusetts Right To Know

Remarks

No components are subject to the Massachusetts Right to Know Act.

#### Pennsylvania Right To Know

*Ingredients*

(4-carboxybutyl)triphenylphosphonium bromide

#### New Jersey Right To Know

*Ingredients*

(4-carboxybutyl)triphenylphosphonium bromide

#### California Prop 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

#### Notification status

TSCA:

Not Listed on TSCA inventory. For Research and Development Use only. Not For Manufacturing or Commercial Purposes.

DSL:

All components of this product are on the Canadian DSL.

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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).

Revision Date 12/12/2012

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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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