

## SAFETY DATA SHEET

Version 4.9  
Revision Date 05/27/2016  
Print Date 11/02/2018

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product name : *t*BuXPhos Pd G1

Product Number : 708739  
Brand : Aldrich

CAS-No. : 1142811-12-8

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

Identified uses : Laboratory chemicals, Synthesis of substances

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

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

#### 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

### 2. HAZARDS IDENTIFICATION

#### 2.1 Classification of the substance or mixture

##### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Carcinogenicity (Category 2), H351  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

For the full text of the H-Statements mentioned in this Section, see Section 16.

#### 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word : Warning

Hazard statement(s)

H315 Causes skin irritation.  
H319 Causes serious eye irritation.  
H335 May cause respiratory irritation.  
H351 Suspected of causing cancer.

Precautionary statement(s)

P201 Obtain special instructions before use.  
P202 Do not handle until all safety precautions have been read and understood.  
P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.  
P264 Wash skin thoroughly after handling.

P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ eye protection/ face protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P321	Specific treatment (see supplemental first aid instructions on this label).
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.2 Mixtures

Synonyms : (t-BuXPhos) palladium(II) phenethylamine chloride  
[2-Di(tert-butylphosphino)-2',4',6'-triisopropyl-1,1'-biphenyl][2-(2-aminoethyl)phenyl]palladium(II) chloride  
t-BuXPhos Palladacycle  
t-BuXPhos precatalyst

Formula : C<sub>37</sub>H<sub>55</sub>ClNPPd

Molecular weight : 686.69 g/mol

#### Hazardous components

Component	Classification	Concentration
<b>T-Buxphos palladium(II) phenethylamine chloride</b>		
CAS-No. 1142811-12-8	Skin Irrit. 2; Eye Irrit. 2A; Carc. 2; STOT SE 3; H315, H319, H335, H351	>= 90 - <= 100 %
<b>tert-Butyl methyl ether</b>		
CAS-No. 1634-04-4	Flam. Liq. 2; Skin Irrit. 2; H225, H315	>= 5 - < 10 %
EC-No. 216-653-1		
Index-No. 603-181-00-X		

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data available

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### 5. FIREFIGHTING MEASURES

#### 5.1 Extinguishing media

##### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

No data available

#### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### 5.4 Further information

No data available

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### 6. ACCIDENTAL RELEASE MEASURES

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

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

#### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

#### 6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

#### 6.4 Reference to other sections

For disposal see section 13.

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### 7. HANDLING AND STORAGE

#### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

#### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Handle and store under inert gas. Air sensitive.

#### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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### 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

#### 8.1 Control parameters

##### Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
tert-Butyl methyl ether	1634-04-4	TWA	50.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Upper Respiratory Tract irritation Kidney damage Confirmed animal carcinogen with unknown relevance to humans		

		PEL	40 ppm 144 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
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Hazardous components without workplace control parameters

## 8.2 Exposure controls

### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

### Personal protective equipment

#### Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

#### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

#### Body Protection

Impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

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|---|--|
| a) Appearance                                   | Form: solid                                      |
| b) Odour  | No data available                                |
| c) Odour Threshold                              | No data available                                |
| d) pH   | No data available                                |
| e) Melting point/freezing point                 | Melting point/range: 150 - 159 °C (302 - 318 °F) |
| f) Initial boiling point and boiling range      | No data available                                |
| g) Flash point                                  | No data available                                |
| h) Evaporation rate                             | No data available                                |
| i) Flammability (solid, gas)                    | No data available                                |
| j) Upper/lower flammability or explosive limits | No data available                                |
| k) Vapour pressure                              | No data available                                |
| l) Vapour density                               | No data available                                |
| m) Relative density                             | No data available                                |
| n) Water solubility                             | No data available                                |
| o) Partition coefficient: n-octanol/water       | No data available                                |

- |                              |                   |
|------------------------------|-------------------|
| p) Auto-ignition temperature | No data available |
| q) Decomposition temperature | No data available |
| r) Viscosity                 | No data available |
| s) Explosive properties      | No data available |
| t) Oxidizing properties      | No data available |

## **9.2 Other safety information**

No data available

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## **10. STABILITY AND REACTIVITY**

### **10.1 Reactivity**

No data available

### **10.2 Chemical stability**

Stable under recommended storage conditions.

### **10.3 Possibility of hazardous reactions**

No data available

### **10.4 Conditions to avoid**

No data available

### **10.5 Incompatible materials**

Oxidizing agents, Strong oxidizing agents, Strong acids

### **10.6 Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Oxides of phosphorus, Hydrogen chloride gas

Other decomposition products - No data available

In the event of fire: see section 5

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## **11. TOXICOLOGICAL INFORMATION**

### **11.1 Information on toxicological effects**

#### **Acute toxicity**

No data available

Inhalation: No data available

Dermal: No data available

No data available

#### **Skin corrosion/irritation**

No data available

#### **Serious eye damage/eye irritation**

No data available

#### **Respiratory or skin sensitisation**

No data available

#### **Germ cell mutagenicity**

No data available

#### **Carcinogenicity**

#### **Reproductive toxicity**

No data available

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

Central nervous system depression, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

Central nervous system - (tert-Butyl methyl ether)

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**12. ECOLOGICAL INFORMATION****12.1 Toxicity**

No data available

**12.2 Persistence and degradability**

No data available

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**12.6 Other adverse effects**

No data available

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**13. DISPOSAL CONSIDERATIONS****13.1 Waste treatment methods****Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

**Contaminated packaging**

Dispose of as unused product.

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**14. TRANSPORT INFORMATION****DOT (US)**

Not dangerous goods

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

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**15. REGULATORY INFORMATION****SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**

The following components are subject to reporting levels established by SARA Title III, Section 313:

tert-Butyl methyl ether	CAS-No. 1634-04-4	Revision Date 2007-07-01
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#### **SARA 311/312 Hazards**

Acute Health Hazard, Chronic Health Hazard

#### **Massachusetts Right To Know Components**

tert-Butyl methyl ether	CAS-No. 1634-04-4	Revision Date 2007-07-01
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#### **Pennsylvania Right To Know Components**

T-Buxphos palladium(II) phenethylamine chloride	CAS-No. 1142811-12-8	Revision Date
tert-Butyl methyl ether	1634-04-4	2007-07-01

#### **New Jersey Right To Know Components**

T-Buxphos palladium(II) phenethylamine chloride	CAS-No. 1142811-12-8	Revision Date
tert-Butyl methyl ether	1634-04-4	2007-07-01

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## **16. OTHER INFORMATION**

### **Full text of H-Statements referred to under sections 2 and 3.**

Carc.	Carcinogenicity
Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H351	Suspected of causing cancer.
Skin Irrit.	Skin irritation
STOT SE	Specific target organ toxicity - single exposure

### **HMIS Rating**

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	0
Physical Hazard	0

### **NFPA Rating**

Health hazard:	2
Fire Hazard:	0
Reactivity Hazard:	0

### **Further information**

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### **Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

Version: 4.9

Revision Date: 05/27/2016

Print Date: 11/02/2018