

## SAFETY DATA SHEET

Version 5.18  
Revision Date 01/08/2018  
Print Date 11/03/2018

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**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : XPhos Pd G1

Product Number : 704954

Brand : Aldrich

CAS-No. : 1028206-56-5

**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)

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**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

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

Acute aquatic toxicity (Category 3), H402

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.

H402

Harmful to aquatic life.

Precautionary statement(s)

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.

P273

Avoid release to the environment.

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.
P312	Call a POISON CENTER/doctor if you feel unwell.
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 : Chloro(2-dicyclohexylphosphino-2',4',6'-triisopropyl-1,1'-biphenyl)[2-(2-aminoethyl)phenyl]palladium(II)  
(2-Dicyclohexylphosphino-2',4',6'-triisopropyl-1,1'-biphenyl)[2-(2-aminoethyl)phenyl]palladium(II) chloride  
(XPhos) palladium(II) phenethylamine chloride  
XPhos Palladacycle  
XPhos precatalyst

Formula : C<sub>41</sub>H<sub>59</sub>ClNPPd

Molecular weight : 738.76 g/mol

#### Hazardous components

Component	Classification	Concentration
<b>Chloro(2-dicyclohexylphosphino-2',4',6'-triisopropyl-1,1'-biphenyl)[2-(2-aminoethyl)phenyl]palladium(II)</b>		
CAS-No. 1028206-56-5	Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H315, H319, H335	90 - 100 %
<b>n-Pentane</b>		
CAS-No. 109-66-0	Flam. Liq. 1; STOT SE 3; Asp.	5 - 10 %
EC-No. 203-692-4	Tox. 1; Aquatic Acute 2;	
Index-No. 601-006-00-1	Aquatic Chronic 2; H224, H304, H336, H411	
<b>tert-Butyl methyl ether</b>		
CAS-No. 1634-04-4	Flam. Liq. 2; Skin Irrit. 2;	5 - 10 %
EC-No. 216-653-1	H225, H315	
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. Discharge into the environment must be avoided.

**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.

Storage class (TRGS 510): 13: Non Combustible Solids

**7.3 Specific end use(s)**

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

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
n-Pentane	109-66-0	TWA	120.000000 ppm 350.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		C	610.000000 ppm 1,800.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
	Remarks	15 minute ceiling value		
		TWA	1,000.000000 ppm 2,950.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	600.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Peripheral neuropathy Adopted values or notations enclosed are those for which changes are proposed in the NIC See Notice of Intended Changes (NIC)		
		TWA	1,000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		narcosis respiratory tract irritation 2017 Adoption		
		PEL	600 ppm 1,800 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
tert-Butyl methyl ether	1634-04-4	TWA	50.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Upper Respiratory Tract irritation Kidney damage Confirmed animal carcinogen with unknown relevance to humans		
		PEL	40 ppm 144 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

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.

Full contact  
Material: Nitrile rubber  
Minimum layer thickness: 0.11 mm  
Break through time: 480 min  
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact  
Material: Nitrile rubber  
Minimum layer thickness: 0.11 mm  
Break through time: 480 min  
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

#### **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**

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. 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. Discharge into the environment must be avoided.

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## **9. PHYSICAL AND CHEMICAL PROPERTIES**

### **9.1 Information on basic physical and chemical properties**

- |                                                 |                                                  |
|-------------------------------------------------|--------------------------------------------------|
| 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: 205 - 210 °C (401 - 410 °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

Strong oxidizing agents

### 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

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

**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

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 (n-Pentane)

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**

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Harmful to aquatic life.

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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.

**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:

	CAS-No.	Revision Date
tert-Butyl methyl ether	1634-04-4	2007-07-01

#### **SARA 311/312 Hazards**

Acute Health Hazard, Chronic Health Hazard

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

	CAS-No.	Revision Date
n-Pentane	109-66-0	1993-04-24
tert-Butyl methyl ether	1634-04-4	2007-07-01

#### **Pennsylvania Right To Know Components**

	CAS-No.	Revision Date
Chloro(2-dicyclohexylphosphino-2',4'6'-triisopropyl-1,1'-biphenyl)[2-(2-aminoethyl)phenyl]palladium(II)	1028206-56-5	
n-Pentane	109-66-0	1993-04-24
tert-Butyl methyl ether	1634-04-4	2007-07-01

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

	CAS-No.	Revision Date
Chloro(2-dicyclohexylphosphino-2',4'6'-triisopropyl-1,1'-biphenyl)[2-(2-aminoethyl)phenyl]palladium(II)	1028206-56-5	
n-Pentane	109-66-0	1993-04-24
tert-Butyl methyl ether	1634-04-4	2007-07-01

#### **California Prop. 65 Components**

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

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## **16. OTHER INFORMATION**

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

Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Asp. Tox.	Aspiration hazard
Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H224	Extremely flammable liquid and vapour.
H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
H402	Harmful to aquatic life.
H411	Toxic to aquatic life with long lasting effects.
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

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