• SAFETY DATA SHEET

Version 6.7
Revision Date 12/25/2025
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SECTION 1. 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

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Skin irritation : Category 2

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Eye irritation	:	Category 2A
Specific target organ toxicity - single exposure	:	Category 3 (Respiratory system)
Short-term (acute) aquatic hazard	:	Category 3
Long-term (chronic) aquatic hazard	:	Category 3

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal word : Warning

Hazard statements : H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.
H412 Harmful to aquatic life with long lasting effects.

Precautionary statements :

Prevention:

P261 Avoid breathing dust.
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.

Response:

P302 + P352 IF ON SKIN: Wash with plenty of water.
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P332 + P313 If skin irritation occurs: Get medical advice/ attention.
P337 + P313 If eye irritation persists: Get medical advice/ attention.

Storage:

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P405 Store locked up.

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Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 1028206-56-5

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Chloro(2-dicylohexylphosphino-2',4'6'-triisopropyl-1,1'-biphenyl)[2-(2-aminoethyl)phenyl]palladium(II)	1028206-56-5*	>= 80 - <= 100	TSC
pentane	109-66-0*	>= 5 - <= 10	TSC
tert-butyl methyl ether	1634-04-4*	>= 5 - <= 10	TSC

* Indicates that the identifier is a CAS No.
TSC- the actual concentration or concentration range is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air.

In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact : After eye contact: rinse out with plenty of water.
Call in ophthalmologist.
Remove contact lenses.

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

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

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Protection of first-aiders	:	For personal protection see section 8.
Notes to physician	:	No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	:	Water Foam Carbon dioxide (CO2) Dry powder
Unsuitable extinguishing media	:	For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	:	Combustible. Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion products	:	Carbon oxides Nitrogen oxides (NOx) Oxides of phosphorus Hydrogen chloride gas
Specific extinguishing methods	:	No data available
Further information	:	Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
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.

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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. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	:	Do not let product enter 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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Further information on storage conditions	:	Tightly closed. Dry.
Storage class	:	11, Combustible Solids
Recommended storage temperature	:	Recommended storage temperature see product label.
Further information on storage stability	:	Handle and store under inert gas. Air sensitive.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
pentane	109-66-0	C	610 ppm 1,800 mg/m3	NIOSH REL
		TWA	120 ppm 350 mg/m3	NIOSH REL
		TWA	1,000 ppm 2,950 mg/m3	OSHA Z-1

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		TWA	1,000 ppm	ACGIH
tert-butyl methyl ether	1634-04-4	TWA	50 ppm	ACGIH

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type P2

The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Material	:	Nitrile rubber
Break through time	:	480 min
Glove thickness	:	0.11 mm
Protective index	:	Full contact
Manufacturer	:	Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Material	:	Nitrile rubber
Break through time	:	480 min
Glove thickness	:	0.11 mm
Protective index	:	Splash contact
Manufacturer	:	Dermatril® (KCL 740 / Aldrich Z677272, Size M)

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

Remarks : 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.
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

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		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.
Eye protection	:	Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses
Skin and body protection	:	protective clothing
Hygiene measures	:	Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	:	solid
Color	:	No data available
Odor	:	No data available
Odor Threshold	:	No data available
pH	:	No data available
Melting point/ range	:	401 - 410 °F / 205 - 210 °C
Boiling point/boiling range	:	No data available
Flash point	:	No data available
Evaporation rate	:	No data available
Flammability (solid, gas)	:	No data available
Flammability (liquids)	:	No data available
Burning rate	:	No data available
Upper explosion limit / Upper flammability limit	:	No data available
Lower explosion limit / Lower flammability limit	:	No data available
Vapor pressure	:	No data available

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Relative vapour density	:	No data available
Relative density	:	No data available
Density	:	No data available
Water solubility	:	No data available
Partition coefficient: n-octanol/water	:	No data available
Autoignition temperature	:	No data available
Decomposition temperature	:	No data available
Viscosity, dynamic	:	No data available
Viscosity, kinematic	:	No data available
Flow time	:	No data available
Explosive properties	:	Not classified as explosive.
Oxidizing properties	:	none
Molecular weight	:	738.76 g/mol
Particle characteristics Particle size	:	No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	:	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	:	The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	:	No data available
Conditions to avoid	:	no information available
Incompatible materials	:	Strong oxidizing agents
Hazardous decomposition	:	In the event of fire: see section 5

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SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
Oral: No data available
Acute toxicity estimate Oral - > 5,000 mg/kg
(Calculation method)

Inhalation: No data available

Acute toxicity estimate Inhalation - 4 h - > 200 mg/l - vapour(Calculation method)

Dermal: No data available

Acute toxicity estimate Dermal - > 5,000 mg/kg
(Calculation method)
No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity

IARC: 2B - Group 2B: Possibly carcinogenic to humans (tert-butyl methyl ether)

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

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.
Stomach - Irregularities - Based on Human Evidence

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SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Product:

Toxicity to fish : Remarks: No data available

Components:

Chloro(2-dicylohexylphosphino-2',4'6'-triisopropyl-1,1'-biphenyl)[2-(2-aminoethyl)phenyl]palladium(II):

Toxicity to fish : Remarks: No data available

pentane:

Toxicity to fish : LC50 (Oncorhynchus mykiss (rainbow trout)): 4.26 mg/l
End point: mortality
Exposure time: 96 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 203
GLP: yes

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 2.7 mg/l
Exposure time: 48 h
Test Type: static test
Analytical monitoring: yes
Remarks: (ECHA)

Toxicity to algae/aquatic plants : ErC50 (Selenastrum capricornutum (green algae)): 10.7 mg/l
Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 201
GLP: yes

NOEC (Selenastrum capricornutum (green algae)): 7.51 mg/l
Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 201
GLP: yes

Ecotoxicology Assessment

Chronic aquatic toxicity : Toxic to aquatic life with long lasting effects.

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tert-butyl methyl ether:

Toxicity to fish	:	LC50 (Menidia beryllina): 574 mg/l End point: mortality Exposure time: 96 h Test Type: semi-static test Analytical monitoring: yes Method: OECD Test Guideline 203
Toxicity to daphnia and other aquatic invertebrates	:	EC50 (Americamysis bahia (Mysid)): 187 mg/l End point: Swimming behavior Exposure time: 96 h Test Type: flow-through test Analytical monitoring: yes Method: US-EPA OPPTS 850.1035 GLP: yes
Toxicity to algae/aquatic plants	:	IC50 (Pseudokirchneriella subcapitata (green algae)): 491 mg/l Exposure time: 96 h Test Type: static test Analytical monitoring: yes GLP: yes
Toxicity to fish (Chronic toxicity)	:	NOEC (Pimephales promelas (fathead minnow)): 299 mg/l End point: Growth inhibition Exposure time: 31 d Test Type: flow-through test Analytical monitoring: yes GLP: yes Remarks: (ECHA) NOEC (Pimephales promelas (fathead minnow)): 450 mg/l End point: mortality Exposure time: 31 d Test Type: flow-through test Analytical monitoring: yes GLP: yes Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	:	NOEC (Daphnia magna (Water flea)): 51 mg/l Exposure time: 21 d Test Type: flow-through test Analytical monitoring: yes Method: OPPTS 850.1300 GLP: yes
Toxicity to microorganisms	:	EC10 (Pseudomonas putida): 710 mg/l End point: Growth rate

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Exposure time: 18 h
Test Type: static test
GLP: yes
Remarks: (ECHA)

Persistence and degradability

Product:

Biodegradability : Remarks: No data available

Components:

Chloro(2-dicylohexylphosphino-2',4'6'-triisopropyl-1,1'-biphenyl)[2-(2-aminoethyl)phenyl]palladium(II):

Biodegradability : Remarks: No data available

pentane:

Biodegradability : aerobic
Inoculum: activated sludge
Concentration: 60 mg/l
Result: Readily biodegradable.
Biodegradation: 87 %
Exposure time: 28 d
Method: OECD Test Guideline 301F
GLP: yes

tert-butyl methyl ether:

Biodegradability : aerobic
Inoculum: activated sludge
Concentration: 2 mg/l
Result: Not readily biodegradable.
Biodegradation: 0 %
Exposure time: 28 d
Method: OECD Test Guideline 301D
GLP: yes

Bioaccumulative potential

Product:

Bioaccumulation : Remarks: No data available

Components:

pentane:

Bioaccumulation : Remarks: No data available

Partition coefficient: n-octanol/water : log Pow: 3.45 (77 °F / 25 °C)
pH: 7
Remarks: Bioaccumulation is not expected.

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tert-butyl methyl ether:

Bioaccumulation	:	Species: Cyprinus carpio (Carp) Bioconcentration factor (BCF): 1.5 Exposure time: 28 d Temperature: 77 °F / 25 °C
Partition coefficient: n-octanol/water	:	log Pow: 1.06 (68 °F / 20 °C) pH: 7 Method: OECD Test Guideline 107 Remarks: Bioaccumulation is not expected.

Mobility in soil

Product:

Stability in soil	:	Remarks: No data available

Other adverse effects

Components:

Chloro(2-dicylohexylphosphino-2',4'6'-triisopropyl-1,1'-biphenyl)[2-(2-aminoethyl)phenyl]palladium(II):

Additional ecological information	:	No data available

pentane:

Additional ecological information	:	Avoid release to the environment. Do not empty into drains.

tert-butyl methyl ether:

Results of PBT and vPvB assessment	:	Not persistent, bioaccumulative, and toxic (PBT). Not very persistent and very bioaccumulative (vPvB).
	:	Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues	:	Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR
Not regulated as a dangerous good

IMDG-Code
Not regulated as a dangerous good

Transport in bulk according to IMO instruments
Not applicable for product as supplied.

National Regulations

49 CFR Road
Not regulated as a dangerous good

Poison Inhalation Hazard : No

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity
Listed substances in the product are at low enough levels to not be expected to exceed the RQ

SARA 304 Extremely Hazardous Substances Reportable Quantity
This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity
This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Acute Health Hazard
Chronic Health Hazard

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

tert-butyl methyl ether	1634-04-4	>= 5 - < 10 %

US State Regulations

Massachusetts Right To Know

pentane	109-66-0
tert-butyl methyl ether	1634-04-4

Pennsylvania Right To Know

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tert-butyl methyl ether	1634-04-4

Maine Chemicals of High Concern

pentane	109-66-0
tert-butyl methyl ether	1634-04-4

Vermont Chemicals of High Concern

pentane	109-66-0

Washington Chemicals of High Concern

pentane	109-66-0

The components of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH	:	USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL	:	USA. NIOSH Recommended Exposure Limits
OSHA Z-1	:	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
ACGIH / TWA	:	8-hour, time-weighted average
NIOSH REL / TWA	:	Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek
NIOSH REL / C	:	Ceiling value not be exceeded at any time.
OSHA Z-1 / TWA	:	8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory;

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LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.
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