



>>Entry Name: Dichlorobis(triphenylphosphine)palladium, 10Cl, 9Cl, 8Cl

Synonym(s): Bis(triphenylphosphine)palladium dichloride

CAS Registry Number: 13965-03-2

$\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$

Molecular Formula: $\text{C}_{36}\text{H}_{30}\text{Cl}_2\text{P}_2\text{Pd}$

Molecular Weight: 701.906

Accurate Mass: 700.023456

Percentage Composition: C 61.60%; H 4.31%; Cl 10.10%; P 8.83%; Pd 15.16%

General Statement: Despite some reports to the contrary, seems to occur only in *trans*-square planar config.

Use/Importance: Mild catalyst in coupling of subst. alkynes and other organomet. reagents. Used in selective carbofunctionalisation of imidazole moiety in L-histidine and its analogues. Also catalyses reaction of 2-bromobenzaldehyde with alkanolamines and CO to give isoindolinones

Aldrich: 41274-0

Fluka: 15253

Sigma: T3764

>>Variant: *cis*-form

CAS Registry Number: 15604-37-2

Molecular Formula: $\text{C}_{36}\text{H}_{30}\text{Cl}_2\text{P}_2\text{Pd}$

Molecular Weight: 701.906

Accurate Mass: 700.023456

Percentage Composition: C 61.60%; H 4.31%; Cl 10.10%; P 8.83%; Pd 15.16%

Other Data: Not separately characterised

>>Variant: *trans*-form

CAS Registry Number: 28966-81-6

Molecular Formula: $\text{C}_{36}\text{H}_{30}\text{Cl}_2\text{P}_2\text{Pd}$

Molecular Weight: 701.906

Accurate Mass: 700.023456

Percentage Composition: C 61.60%; H 4.31%; Cl 10.10%; P 8.83%; Pd 15.16%

Source/Synthesis: Synth. from $\text{PdCl}_4^{2-} + \text{PPh}_3$, or from $\text{PdCl}_2 + \text{PPh}_3$ melt

Use/Importance: Catalyst for carbonylation of halides to carboxylic acid and amides. Accelerates polymn. of methylpropiolate, leading to prod. with lower cyclic oligomer content. Commercially available

Physical Description: Hygroscopic bright yellow cryst. (toluene)

Melting Point: Mp 297-298 dec.°. Mp 298-300 dec.°

Solubility: Sol. many polar org. solvs.

Other Data: Pd-*o*-H on phenyl ring is short at 292 pm

Hazard & Toxicity: ATP-ase inhibitor

References:

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Grim, S.O., *Inorg. Chim. Acta*, 1970, **4**, 56, (*nmr*)
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Brauer, G., *Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **3**, 2014, (*synth*)
Uson, R. *et al.*, *J. Organomet. Chem.*, 1977, **132**, 429, (*synth*)
MacDougall, J.J. *et al.*, *Inorg. Nucl. Chem. Lett.*, 1979, **15**, 315, (*cmr, P-31 nmr*)
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Simionescu, C.I. *et al.*, *J. Macromol. Sci., Chem.*, 1987, **24**, 611, (*use*)
Evans, D.A. *et al.*, *Angew. Chem., Int. Ed.*, 1993, **32**, 1326, (*use*)
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Cho, C.S. *et al.*, *Synth. Commun.*, 1997, **27**, 4141-4158, (*use, synth of isoindolinones*)