



>>Entry Name: Chlorophenylmercury, 9Cl

Synonym(s): Phenylmercury chloride. Chloromercuribenzene

CAS Registry Number: 100-56-1

PhHgCl

Molecular Formula: C₆H₅ClHg

Molecular Weight: 313.148

Accurate Mass: 313.978594

Percentage Composition: C 23.01%; H 1.61%; Cl 11.32%; Hg 64.06%

Source/Synthesis: Synth. from PhN₂Cl, HgCl₂ and Cu

Use/Importance: Reacts with RCOX in presence of Pd(0); reacts with H₂C=CH[*cyclo*-CHCH₂C(=O)NH] in presence of catalytic Pd^{II} → PhCH₂CH=CHCH₂CONH₂ with reasonable stereoselection; substitutes vinyl halides in presence of catalytic Rh^I, vinyl bromide in presence of Wilkinson's catalyst, acyl halides in presence of AlCl₃ and allyl halides in presence of LiPdCl₃; reacts with stoichiometric Co₂(CO)₈ → Ph₂CO; undergoes stoichiometric Heck reaction with Li₂PdCl₄ and catalytic Heck in presence of Pd, Cu salts; homocouples to biphenyl in presence of Rh^I or Pd^{II}; reacts with elemental S → PhSSPh; undergoes chloroarylation of alkenes in presence of Li₂PdCl₄, LiCl and excess CuCl₂; undergoes catalytic methylation by MeI in presence of RhI₂Me(PPh₃)₂; couples with Li₂CuMe₃ and other organocopper lithium reagents; undergoes conjugate addn. to enones in presence of PdCl₂ under strongly acidic phase transfer conditions; reacts with CO in presence of Li₂PdCl₄/CuCl₂ → Ph₂CO; undergoes radical addn. to alkenes using NaBH₄; adds phenol *trans*- to aryl alkenes in presence of Li₂PdCl₄ aq.

Biological Use/Importance: Bactericide

Physical Description: Plates (C₆H₆)

Melting Point: Mp 258° (251°)

Solubility: Spar. sol. EtOH, C₆H₆; insol. H₂O

Other Data: Sublimes

Hazard & Toxicity: LD₅₀ (rat, orl) 60 mg/kg. LD₅₀ (rat, scu) 47 mg/kg

Aldrich: P2713-5

Fluka: 79132

References:

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