



>>Entry Name: Dichlorobis(η^5 -2,4-cyclopentadien-1-yl)zirconium, 9Cl

Synonym(s): Zirconocene dichloride. Bis(cyclopentadienyl)zirconium chloride

CAS Registry Number: 1291-32-3

BB0240 BB0260 BB0300 BB0332 BB0390

As Dibromobis(η^5 -2,4-cyclopentadien-1-yl)zirconium, BQC50-P with
X = Y = Cl

Molecular Formula: C₁₀H₁₀Cl₂Zr

Molecular Weight: 292.318

Accurate Mass: 289.920657

Percentage Composition: C 41.09%; H 3.45%; Cl 24.26%; Zr 31.21%

Source/Synthesis: synth. from ZrCl₄ + LiCp

Use/Importance: Precursor to Cp₂Zr(*II* or *IV*) compds. Catalyses aldol/Nazarov reactions of ketones with aldehydes → cyclopentenones; cyclotrimerises cyclohexanone, cyclopentanone to annelated benzenes; used in rearrangement reactions of epoxy esters; catalyst for isom. and regioselective terminal hydrosilylation of alkenes; for hydrogenation of alkenes, alkynes; for isom. of allyl benzene; and for epoxidn. of cyclohexene; catalyses S_N2' subst. of allyl ethers by Grignard reagents; carbometallation of alkenes, alkynes; alkene polym. with methylaluminoxane. Effects dimerisation of aldehydes to esters. With Bu^tMgCl, reagent for hydrozirconation of simple alkenes and carbazirconation of styrene, dienes. Used in prep. of zirconium enolates. With AgClO₄ effects glycosidation of glycosyl fluorides with a range of alcohols. With Zn/CH₂X₂, reagent for methylenation of aldehydes, ketones, enones. Used in synth. of phospholes from RPCl₂ and alkynes. Catalyses cross-aromatisation of cyclohexanones with RCHO → 2,6-bis(CH₂R)phenol. Catalyst for stereo- and regio-selective alkylation of unsatd. compds. Effects the coupling of EtMgBr, alkynes and CO giving cyclopentenones; catalyses the selective dehalogenation of aromatic halides by Grignard reagents

Biological Use/Importance: Has antitumour activity

Physical Description: Colourless cryst.

Melting Point: Mp 248° (242-245°)

Boiling Point: Subl. 150-180°

Aldrich: 19621-5

Fluka: 14693

Rare Chemicals Library: S41657-6

Sigma: Z0542

References: