



>>Entry Name: Bis(η^5 -2,4-cyclopentadien-1-yl)dimethylzirconium, 10Cl

Synonym(s): Zirconocene dimethyl

CAS Registry Number: 12636-72-5

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

Molecular Formula: C₁₂H₁₆Zr

Molecular Weight: 251.482

Accurate Mass: 250.029903

Percentage Composition: C 57.31%; H 6.41%; Zr 36.27%

Source/Synthesis: Synth. from ZrCp₂Cl₂ and MeLi in Et₂O

Use/Importance: Cocatalyst in metathesis reactions; catalyses polym. of Me₃SiSiHMe₂ and relat. compds.; with [Cp₂ZrMe(THF)]BPh₄ or methylaluminoxane, catalyses polym. of alkenes; adds to aldehydes and ketones in the presence of KOBu^t; adds to ketenes, isocyanates and carbodiimides

Physical Description: White cryst. (by subl.)

Boiling Point: Subl._{-0.0001} 60-80°

Other Data: Isotopomers studied

References:

Samuel, E. *et al.*, *J.A.C.S.*, 1973, **95**, 6263, (*synth, nmr*)

Alt, H. *et al.*, *J.A.C.S.*, 1974, **96**, 5936

Jordan, R.F. *et al.*, *J.A.C.S.*, 1979, **101**, 4853, (*cmr*)

Ger. Pat., 1981, 3 007 725; *CA*, **95**, 187927j, (*use*)

Van Leeuwen, P.W.N.M. *et al.*, *J. Organomet. Chem.*, 1981, **209**, 169, (*cidnp*)

McQuillan, G.P. *et al.*, *J. Organomet. Chem.*, 1986, **312**, 183, (*ir*)

Negishi, E. *et al.*, *Synthesis*, 1988, 1, (*use, addn reactions*)

Hengge, E. *et al.*, *J. Organomet. Chem.*, 1991, **410**, C1, (*use, polym of silanes*)

Larson, A.L. *et al.*, *Tet. Lett.*, 1991, **32**, 5893, (*use, reaction with aldehydes, ketones*)

Sishta, C. *et al.*, *J.A.C.S.*, 1992, **114**, 1112, (*use, polym of alkenes*)

Collins, S. *et al.*, *J.A.C.S.*, 1992, **114**, 5460, (*use, polym of alkenes*)