



>>Entry Name: Zirconium isopropoxide

Synonym(s): 2-Propanol zirconium(4+) salt, 9Cl. Isopropyl orthozirconate. Isopropyl zirconate(IV). Tetraisopropyl zirconate

CAS Registry Number: 2171-98-4



Molecular Formula: $\text{C}_{12}\text{H}_{28}\text{O}_4\text{Zr}$

Molecular Weight: 327.575

Accurate Mass: 326.103463

Percentage Composition: C 44.00%; H 8.62%; O 19.54%; Zr 27.85%

Source/Synthesis: Synth. from ZrCl_4 and Pr^iOH ; the Pr^iOH solvate obt. is purified and heated to remove Pr^iOH and the residue distilled; also synth. from ZrCl_4 and NaOPr^i

Use/Importance: Commercially available. Precursor to other useful Zr reagents; hydrogenation catalyst; catalyses selective Meerwein-Ponndorf-Verley redn. and Oppenauer oxidn.; used in ester synth.; effects dimerisation of amino acids to form diketopiperazines

Physical Description: Moisture-sensitive liq.

Boiling Point: $\text{Bp}_{0.1}$ 160°

Solubility: Readily sol. org. solvs.

>>Derivative: 2-Propanol solvate (1:1), dimer

CAS Registry Number: 146262-17-1

Extra CAS Registry Numbers(s): 50939-84-9

Molecular Formula: $\text{C}_{30}\text{H}_{72}\text{O}_{10}\text{Zr}_2$

Molecular Weight: 775.341

Accurate Mass: 772.321956

Percentage Composition: C 46.47%; H 9.36%; O 20.64%; Zr 23.53%

Source/Synthesis: Obt. by recryst. of crude $\text{Zr}(\text{OPr}^i)_4$ from Pr^iOH

Physical Description: White cryst. (2-propanol)

Melting Point: Mp 138-141°

Solubility: Spar. sol. 2-propanol

References:

Bradley, D.C. *et al.*, *J.C.S.*, 1951, 280, (*synth*)

Inorg. Chim. Acta, 1981, **53**, L73-L76

Shreider, V.A. *et al.*, *Inorg. Chim. Acta*, 1981, **53**, L73-L76, (*solvate, synth*)

Japan. Pat., 1985, 60 258 132; *CA*, **105**, 26611m, (*manuf*)

Nakano, T. *et al.*, *J.O.C.*, 1987, **52**, 4855-4859, (*synth, ir, pmr, cmr*)

Eur. Pat., 1989, 299 171; *CA*, **111**, 38866k, (*manuf*)

Vaartstra, B.A. *et al.*, *Inorg. Chem.*, 1990, **29**, 3126-3131, (*solvate, synth, ir, pmr, cmr, cryst struct*)

Gundersen, L.-L. *et al.*, *Encyclopaedia of Reagents for Organic Synthesis*, (ed. Paquette, L.A.), Wiley, 1995, **8**, 5581-5582, (*synth, use*)