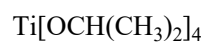




>>Entry Name: Titanium(IV) isopropoxide

Synonym(s): Titanium(IV) tetraisopropoxide. Tetraisopropyl titanate. Isopropyl titanate(IV). Isopropyl orthotitanate. 2-Propanol titanium(4+) salt, 12Cl. Isopropyl alcohol titanium(4+) salt, 8Cl

CAS Registry Number: 546-68-9



Molecular Formula: C₁₂H₂₈O₄Ti

Molecular Weight: 284.231

Accurate Mass: 284.146707

Percentage Composition: C 50.71%; H 9.93%; O 22.52%; Ti 16.85%

Use/Importance: Commercially available. Used in a catalytic system for fixing dinitrogen; polym. catalyst. Mild Lewis acid, used as a catalyst in transesterification reactions, nucleophilic cleavages of 2,3-epoxyalcohols and isomerisations; additive in the Sharpless epoxidation and in nucleophilic addns. to carbonyl and α,β -unsatd. carbonyl compds. Selectively cleaves allyl ethers and carboxylates in the presence of CyMgCl or BuMgCl

Physical Description: Liq. or low-melting solid

Melting Point: Mp 18-20°

Boiling Point: Bp 220°. Bp₁₀ 101-104°. Bp₁₀ 218°

Solubility: Sol. many solvs. including ethers, org. halides, alcohols, C₆H₆

Hazard & Toxicity: Irritant; flammable. Fl. p. 25°. LD₅₀ (rat,ihl) 7.78 mg/kg

Aldrich: 37799-6

Fluka: 87560

Other: Gelest AKT872

References:

Bradley, D.C. *et al.*, *J.C.S.*, 1952, 5020, (*synth*)

Kriegsmann, H. *et al.*, *Z. Elektrochem.*, 1958, **62**, 1163, (*ir, Raman*)

Bradley, D.C. *et al.*, *CA*, 1965, **63**, 7794, (*pmr*)

Holloway, C.E., *J.C.S. Dalton*, 1976, 1050, (*cmr*)

Babonneau, F. *et al.*, *Inorg. Chem.*, 1988, **27**, 3166, (*struct by xanes and xafs*)

Traill, P.R. *et al.*, *J. Magn. Reson.*, 1990, **90**, 551, (*Ti-49 nmr*)

Banwell, M.G., *Encyclopaedia of Reagents for Organic Synthesis*, (ed. Paquette, L.A.), Wiley, 1995, **7**, 4932, (*use*)

Lee, J. *et al.*, *Tet. Lett.*, 1996, **37**, 3663, (*use, cleavage of ethers, carboxylates*)

U.S. Pat., 3 119 852; *CA*, **60**, 11898, (*synth*)

Sax, N.I., *Dangerous Properties of Industrial Materials*, 5th edn., Van Nostrand Reinhold, 1979, 1018