



>>Entry Name: Aluminium *tert*-butoxide

Synonym(s): 2-Methyl-2-propanol aluminium salt, 9CI. *tert*-Butyl alcohol aluminium salt, 8CI. Aluminium 2-methyl-2-propoxide

CAS Registry Number: 556-91-2

$\text{Al}[\text{OC}(\text{CH}_3)_3]_3$

Molecular Formula: $\text{C}_{12}\text{H}_{27}\text{AlO}_3$

Molecular Weight: 246.325

Accurate Mass: 246.177559

Percentage Composition: C 58.51%; H 11.05%; Al 10.95%; O 19.49%

General Statement: Dimeric in C_6H_6

Other Data: Traces of moisture or alcohols cause melting at 160-200°. $\text{Al}_2(\text{NMe}_2)(\text{OBu}^t)_5$ also descr.

Aldrich: 23584-9

Fluka: 6201

Other: Gelest AKA030

>>Derivative: Dimer

Molecular Formula: $\text{C}_{24}\text{H}_{54}\text{Al}_2\text{O}_6$

Molecular Weight: 492.65

Accurate Mass: 492.355118

Percentage Composition: C 58.51%; H 11.05%; Al 10.95%; O 19.49%

Source/Synthesis: Synth. from $\text{Al}_2(\text{NMe}_2)_6$ and Bu^tOH in C_6H_6

Use/Importance: Condensing agent. Reagent for the Oppenauer oxidn. of alcohols to carbonyl compds.

Physical Description: Colourless cryst. (toluene)

Melting Point: Mp 300° (sealed tube)

Boiling Point: Subl. 180°

>>Derivative: NHMe_2 complex

Molecular Formula: $\text{C}_{14}\text{H}_{34}\text{AlNO}_3$

Molecular Weight: 291.409

Percentage Composition: C 57.70%; H 11.76%; Al 9.26%; N 4.81%; O 16.47%

Physical Description: Moisture-sensitive white cryst. (toluene)

Other Data: Subl._{0.1} 40-50°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1281A, (*ir*)

Mehrotra, R.C., *J. Indian Chem. Soc.*, 1953, **30**, 585, (*synth*)

Coffey, S. *et al.*, *J.C.S.*, 1954, 2468, (*synth*)

Org. Synth., *Coll. Vol.*, 3, 1955, 48, (*synth*)

Shiner, V.J. *et al.*, *J.A.C.S.*, 1963, **85**, 2318, (*pmr, struct*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 23

Kozlova, I.K. *et al.*, *CA*, 1968, **70**, 3179, (*synth*)

Chisholm, M.H. *et al.*, *Inorg. Chem.*, 1991, **30**, 1020, (*synth, cryst struct*)