



>>Entry Name: Lithium *tert*-butoxide

Synonym(s): 2-Methyl-2-propanol lithium salt. *tert*-Butoxylithium

CAS Registry Number: 1907-33-1

$\text{LiOC}(\text{CH}_3)_3$

Molecular Formula: $\text{C}_4\text{H}_9\text{LiO}$

Molecular Weight: 80.055

Accurate Mass: 80.081343

Percentage Composition: C 60.01%; H 11.33%; Li 8.67%; O 19.99%

Source/Synthesis: Synth. from Li metal and Bu^tOH in Et_2O , or from BuLi , Bu^tOH and cyclopropyl carbinol under N_2

Use/Importance: Used as a catalyst in numerous reactions, e.g. polym. of butadiene with styrene, polym. of acrylonitrile. Used as a gelling agent for liq. hydrocarbons

Physical Description: Monoclinic cryst. (Et_2O or hexane)

Boiling Point: $\text{Subl}_{0.01}$ 110°

Solubility: V. sol. most org. solvs.

Other Data: Ir ν_{CH} 2945vs, 2850s; $\nu_{\text{CH}3}$ 1470w, 1375m, 1353s; $\nu_{\text{C-O}}$ 1209vs; $\nu_{\text{CH(rock)}}$ 1013m; ν_{COLi} 970vs; $\nu_{\text{CH}2(\text{rock})}$ 883w; ν_{CC} 748; $\nu_{\text{O-Li}}$ 578vs, 507s; $\nu_{\text{C-C-C}}$ 462m, 395s cm^{-1} . Pmr 6.2 ppm. V. reactive; must be studied under Ar

Aldrich: 40017-3

Fluka: 62467

Other: Gelest AKL454

References:

Siminov, A.P. *et al.*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1961, **136**, 634, (*ir, synth*)

Golovanov, I.B. *et al.*, *Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1963, **149**, 835, (*pmr*)

Huml, K., *Czech. J. Phys.*, 1965, **15**, 699; *CA*, **64**, 4373c, (*struct*)

Hartwell, G.E. *et al.*, *Inorg. Chem.*, 1966, **5**, 1257, (*ms*)

Siminov, A.P. *et al.*, *CA*, 1967, **67**, 86234x, (*ir*)

Scherr, P.A. *et al.*, *J.A.C.S.*, 1974, **96**, 6055, (*Li-7 nmr*)

Ito, H. *et al.*, *Macromolecules*, 1990, **23**, 2589, (*synth*)