



>>Entry Name: **2,6-Di-*tert*-butylphenol**

Synonym(s): 2,6-Bis(1,1-dimethylethyl)phenol, 9CI. Ethyl 701

CAS Registry Number: 128-39-2

Molecular Formula: C₁₄H₂₂O

Molecular Weight: 206.327

Accurate Mass: 206.167065

Percentage Composition: C 81.50%; H 10.75%; O 7.75%

Melting Point: Mp 36.5°

Boiling Point: Bp₃₀ 147°

Hazard & Toxicity: LD₅₀ (mus, ivn) 120 mg/kg

Aldrich: D4840-0

Fluka: 34800

Sigma: D3292

>>Derivative: Phenylurethane

Physical Description: Cryst. (petrol)

Melting Point: Mp 148-150°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 259B, (*nmr*)

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 650H, (*ir*)

Hart, H. *et al.*, *J.A.C.S.*, 1951, **73**, 3179, (*synth*)

Stroh, R. *et al.*, *Angew. Chem.*, 1957, **69**, 699, (*synth*)

Kolka, A.J. *et al.*, *J.O.C.*, 1957, **22**, 642, (*synth*)

Kealy, T.J. *et al.*, *J.O.C.*, 1961, **26**, 987, (*synth*)