



>>Entry Name: 3,5-Di-*tert*-butylphenol

Synonym(s): 3,5-Bis(1,1-dimethylethyl)phenol, 9CI

CAS Registry Number: 1138-52-9

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 92-93.5°

Aldrich: D4850-8

>>Derivative: Benzoyl

CAS Registry Number: 5723-92-2

Molecular Formula: C₂₁H₂₆O₂

Molecular Weight: 310.435

Accurate Mass: 310.19328

Percentage Composition: C 81.25%; H 8.44%; O 10.31%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 82-83°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 262C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1084C, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1017D, (*ir*)

Allinger, N.L. *et al.*, *J.A.C.S.*, 1966, **88**, 2999, (*synth*)

Myhre, P.C. *et al.*, *J.A.C.S.*, 1968, **90**, 2115, (*synth*)

Norell, J.R., *J.O.C.*, 1973, **38**, 1924, (*synth*)