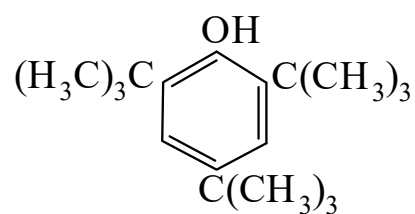




>>Entry Name: 2,4,6-Tri-*tert*-butylphenol, 8Cl

Synonym(s): 2,4,6-Tris(1,1-dimethylethyl)phenol, 9Cl. Alkofen B



CAS Registry Number: 732-26-3

Related CAS Registry Numbers(s): 2525-39-5

Molecular Formula: C₁₈H₃₀O

Molecular Weight: 262.434

Accurate Mass: 262.229665

Percentage Composition: C 82.38%; H 11.52%; O 6.10%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 130-131°

Boiling Point: Bp₁₀ 136°

pKa Value: pK_{a1} 12.19 (25°)

Aldrich: T4940-9

>>Derivative: Benzenesulfonyl

Physical Description: Cryst. (MeOH)

Melting Point: Mp 124.5-126.5°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1095B, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 286A, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1032A, (*ir*)

Stillson, G.H. *et al.*, *J.A.C.S.*, 1945, **67**, 303

Adv. Chem. Ser., 1955, **15**, 322, (*props*)

Sommers, B.G. *et al.*, *J. Chem. Educ.*, 1955, **32**, 312

Bowie, R.A. *et al.*, *Tet. Lett.*, 1968, 5471, (*pmr*)

Musso, H. *et al.*, *Chem. Ber.*, 1969, **102**, 706, (*ir*)

Kahevec, J. *et al.*, *Chem. Ind. (London)*, 1969, 489