



>>Entry Name: 1,3,5-Tri-*tert*-butylbenzene, 8Cl

Synonym(s): 1,3,5-Tris(1,1-dimethylethyl)benzene, 9Cl

CAS Registry Number: 1460-02-2

Molecular Formula: C₁₈H₃₀

Molecular Weight: 246.435

Accurate Mass: 246.23475

Percentage Composition: C 87.73%; H 12.27%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 72-74°

Boiling Point: Bp 248°. Bp₁₂ 121-122°

Aldrich: 22377-8

Fluka: 90793

Sigma: T5533

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 943C, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 20B, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 864A, (*ir*)

Bartlett, P.D. *et al.*, *J.A.C.S.*, 1954, **76**, 2349-2353, (*synth*)

Barclay, L.R.C. *et al.*, *Can. J. Chem.*, 1955, **33**, 672-678, (*synth*)

Dale, J., *Chem. Ber.*, 1961, **94**, 2821-2823, (*uv, ir*)

Myhre, P.C. *et al.*, *J.O.C.*, 1966, **31**, 3425-3426, (*synth*)

Sakai, T., *Acta Cryst. B*, 1978, **34**, 3649, (*cryst struct*)

Ditto, S.R., *J.O.C.*, 1979, **44**, 894-896, (*synth, pmr*)

Synthetic Methods of Organometallic and Inorganic Chemistry, (ed. Hermann, W.A.), Thieme, 1996, **3**, 118-125, (*synth, pmr*)