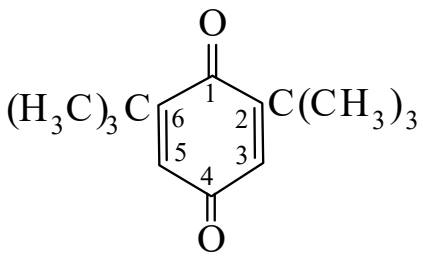
>>**Entry Name: 2,6-Di-*tert*-butyl-1,4-benzoquinone**
ENTRY UNDER REVIEW
Synonym(s): 2,6-Bis(1,1-dimethylethyl)-2,5-cyclohexadiene-1,4-dione, 9CI



CAS Registry Number: 719-22-2

Molecular Formula: $C_{14}H_{20}O_2$
Molecular Weight: 220.311
Accurate Mass: 220.14633
Percentage Composition: C 76.33%; H 9.15%; O 14.52%
Source/Synthesis: Detected in tapwater as presumed oxidant of 2,6-Di-*tert*-butyl-4-methylphenol HCH42-H. Formed as dec. prod. of 2,6-Di-*tert*-butyl-4-methylphenol HCH42-H in fat frying
Physical Description: Yellow cryst. (MeOH)
Melting Point: Mp 68°
Boiling Point: $Subl._{0.01}$ 60°
Hazard & Toxicity: LD_{50} (mus, ipr) 2270 mg/kg

Aldrich: 15393-1

>>**Derivative:** 4-Oxime

CAS Registry Number: 15052-28-5
Molecular Formula: $C_{14}H_{21}NO_2$
Molecular Weight: 235.325
Accurate Mass: 235.157229
Percentage Composition: C 71.46%; H 8.99%; N 5.95%; O 13.60%
Physical Description: Yellow plates (C_6H_6)
Melting Point: Mp 221-222°

>>**Derivative:** 4-(2,4-Dinitrophenylhydrazone)

Physical Description: Red cryst.
Melting Point: Mp 198-200°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 453A, *(ir)*
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 714B, *(nmr)*
Metro, S.J., *J.A.C.S.*, 1955, **77**, 2901, *(synth, deriv)*
Ley, K. *et al.*, *Chem. Ber.*, 1956, **89**, 1402, *(synth)*
Kharasch, M.S. *et al.*, *J.O.C.*, 1962, **27**, 651, *(synth, deriv)*
Heiss, J. *et al.*, *Org. Mass Spectrom.*, 1969, **2**, 1325, *(ms)*
Rieker, A. *et al.*, *Z. Naturforsch., B*, 1969, **24**, 547, *(pmr, uv, ir)*
Berger, S. *et al.*, *Tetrahedron*, 1972, **28**, 3123, *(cmr)*
Kikuchi, T. *et al.*, *Chem. Pharm. Bull.*, 1983, **31**, 659, *(isol)*
Barton, D.H.R. *et al.*, *Synth. Commun.*, 1997, **27**, 3625-3630, *(synth, pmr, cmr)*