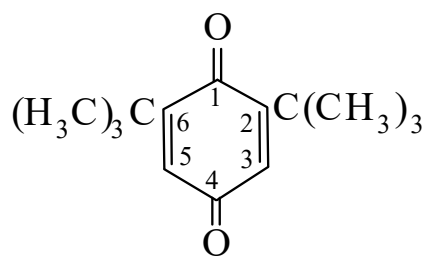




>>Entry Name: 2,6-Di-*tert*-butyl-1,4-benzoquinone

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: C₁₄H₂₀O₂

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: LD₅₀ (mus, ipr) 2270 mg/kg

Aldrich: 15393-1

>>Derivative: 4-Oxime

CAS Registry Number: 15052-28-5

Molecular Formula: C₁₄H₂₁NO₂

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 (C₆H₆)

Melting Point: Mp 221-222°

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

Physical Description: Red cryst.

Melting Point: Mp 198-200°

References:

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Heiss, J. *et al.*, *Org. Mass Spectrom.*, 1969, **2**, 1325, (*ms*)
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