



>>Entry Name: 1,4-Diphenyl-2-butene-1,4-dione, 9CI

Synonym(s): 1,2-Dibenzoylethylene. Diphenacylidene

CAS Registry Number: 4070-75-1

PhCOCH=CHCOPh

Molecular Formula: C₁₆H₁₂O₂

Molecular Weight: 236.27

Accurate Mass: 236.08373

Percentage Composition: C 81.34%; H 5.12%; O 13.54%

>>Variant: (E)-form

CAS Registry Number: 959-28-4

Molecular Formula: C₁₆H₁₂O₂

Molecular Weight: 236.27

Accurate Mass: 236.08373

Percentage Composition: C 81.34%; H 5.12%; O 13.54%

Use/Importance: Dienophile in synthesis

Physical Description: Yellow needles (C₆H₆)

Melting Point: Mp 111°

Aldrich: D3320-9

Fluka: 33560

>>Derivative: Dioxime

Molecular Formula: C₁₆H₁₄N₂O₂

Molecular Weight: 266.299

Accurate Mass: 266.105528

Percentage Composition: C 72.17%; H 5.30%; N 10.52%; O 12.02%

Physical Description: Plates (EtOH aq.)

Melting Point: Mp 202-203°

>>Variant: (Z)-form

CAS Registry Number: 959-27-3

Molecular Formula: C₁₆H₁₂O₂

Molecular Weight: 236.27

Accurate Mass: 236.08373

Percentage Composition: C 81.34%; H 5.12%; O 13.54%

Physical Description: Cryst.

Melting Point: Mp 134°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 875A, (nmr)

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 880D, (ir)

Org. Synth., Coll. Vol., 3, 1955, 248, (synth)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 195

Rio, G. *et al.*, *Bull. Soc. Chim. Fr.*, 1969, 1664, (synth)

Rabinovich, D. *et al.*, *J.C.S.(B)*, 1970, 17, (struct)

Furukawa, J. *et al.*, *Bull. Chem. Soc. Jpn.*, 1976, **49**, 829, (synth)

Bart, J.C.J. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1978, **97**, 231, (struct)

Ohsawa, A. *et al.*, *J.O.C.*, 1979, **44**, 3524, (oxime)