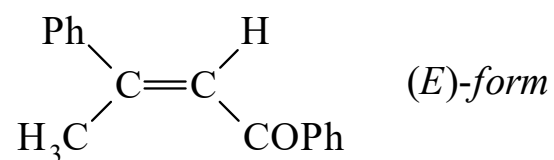




>>Entry Name: **1,3-Diphenyl-2-buten-1-one**, 9CI

Synonym(s): β -Methylchalcone, 8CI. β -Methylstyryl phenyl ketone. β -Benzoyl- α -methylstyrene. Dypnone



CAS Registry Number: 495-45-4

Molecular Formula: C₁₆H₁₄O

Molecular Weight: 222.286

Accurate Mass: 222.104465

Percentage Composition: C 86.45%; H 6.35%; O 7.20%

Boiling Point: Bp 340-345° dec.. Bp₅₀ 246°. Bp₂₂ 225°

Density: d₀²⁰ 1.108

Other Data: Mixt. of approx. 85% (*E*)-form and 15% (*Z*)- as shown by cmr. Isomers photoequilibrate

Hazard & Toxicity: Fl. p. 177° (oc). Eye and skin irritant. LD₅₀ (rat, orl) 3600 mg/kg

Rare Chemicals Library: S37154-8

>>Variant: (*E*)-form

Molecular Formula: C₁₆H₁₄O

Molecular Weight: 222.286

Accurate Mass: 222.104465

Percentage Composition: C 86.45%; H 6.35%; O 7.20%

>>Derivative: Oxime (*E*)-

Molecular Formula: C₁₆H₁₅NO

Molecular Weight: 237.301

Accurate Mass: 237.115364

Percentage Composition: C 80.98%; H 6.37%; N 5.90%; O 6.74%

Physical Description: Needles

Melting Point: Mp 78°

>>Derivative: Oxime (*Z*)-

Molecular Formula: C₁₆H₁₅NO

Molecular Weight: 237.301

Accurate Mass: 237.115364

Percentage Composition: C 80.98%; H 6.37%; N 5.90%; O 6.74%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 134°

>>Derivative: Semicarbazone

Physical Description: Prisms (C₆H₆)

Melting Point: Mp 151°

References:

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