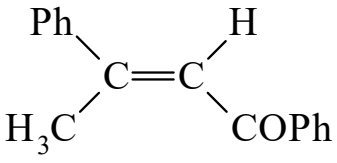
>>**Entry Name: 1,3-Diphenyl-2-buten-1-one,** 9CI

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



(*E*)-*form*

CAS Registry Number: 495-45-4

Molecular Formula: $C_{16}H_{14}O$
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.. Bp_{50} 246°. Bp_{22} 225°
Density: d_0^{20}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. LD_{50} (rat, orl) 3600 mg/kg

Rare Chemicals Library: S37154-8

>>**Variant:** (*E*)-form

Molecular Formula: $C_{16}H_{14}O$
Molecular Weight: 222.286
Accurate Mass: 222.104465
Percentage Composition: C 86.45%; H 6.35%; O 7.20%

>>**Derivative:** Oxime (*E*)-

Molecular Formula: $C_{16}H_{15}NO$
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: $C_{16}H_{15}NO$
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 (C_6H_6)
Melting Point: Mp 151°

References:

Calloway, N.O. *et al.*, *J.A.C.S.*, 1937, **59**, 809, *(synth)*
Black, W.B. *et al.*, *J.A.C.S.*, 1955, **77**, 5134, *(uv)*
Org. Synth., Coll. Vol., 3, 1955, 367, *(synth)*
Uemura, S. *et al.*, *Bull. Chem. Soc. Jpn.*, 1972, **45**, 860, *(synth)*
Rozynov, B.V. *et al.*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1974, **7**, 1602, *(ms)*
Kingsbury, C.A. *et al.*, *J.O.C.*, 1976, **41**, 3863, *(cmr)*
Bouhlel, E. *et al.*, *Synth. Commun.*, 1992, **22**, 2183, *(synth)*
Lewis, R.J.*, Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MPL000