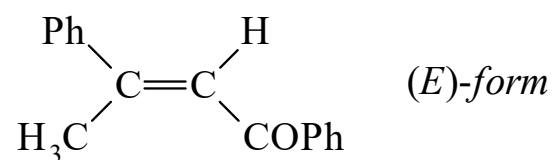




>>Entry Name: **1,3-Diphenyl-2-buten-1-one**, 9CI

Synonym(s):  $\beta$ -Methylchalcone, 8CI.  $\beta$ -Methylstyryl phenyl ketone.  $\beta$ -Benzoyl- $\alpha$ -methylstyrene. Dypnone



CAS Registry Number: 495-45-4

Molecular Formula: C<sub>16</sub>H<sub>14</sub>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<sub>50</sub> 246°. Bp<sub>22</sub> 225°

Density: d<sub>0</sub><sup>20</sup> 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<sub>50</sub> (rat, orl) 3600 mg/kg

Rare Chemicals Library: S37154-8

>>Variant: (*E*)-form

Molecular Formula: C<sub>16</sub>H<sub>14</sub>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<sub>16</sub>H<sub>15</sub>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<sub>16</sub>H<sub>15</sub>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<sub>6</sub>H<sub>6</sub>)

Melting Point: Mp 151°

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