



>>Entry Name: **1,2-Diphenyl-1-butanone**

**Synonym(s):** 2-Phenylbutyrophenone. 1-Benzoyl-1-phenylpropane

**CAS Registry Number:** 16282-16-9

H3CCH2CHPhCOPh

**Molecular Formula:** C<sub>16</sub>H<sub>16</sub>O

**Molecular Weight:** 224.302

**Accurate Mass:** 224.120115

**Percentage Composition:** C 85.68%; H 7.19%; O 7.13%

**Aldrich:** 27747-9

**Rare Chemicals Library:** S32773-5

>>Variant: (+)-form

**Molecular Formula:** C<sub>16</sub>H<sub>16</sub>O

**Molecular Weight:** 224.302

**Accurate Mass:** 224.120115

**Percentage Composition:** C 85.68%; H 7.19%; O 7.13%

**Physical Description:** Cryst. (EtOH/pentane)

**Melting Point:** Mp 57-58°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>25</sup>+230.2 (c, 4.99 in C<sub>6</sub>H<sub>6</sub>)

>>Variant: (±)-form

**CAS Registry Number:** 77542-11-1

**Molecular Formula:** C<sub>16</sub>H<sub>16</sub>O

**Molecular Weight:** 224.302

**Accurate Mass:** 224.120115

**Percentage Composition:** C 85.68%; H 7.19%; O 7.13%

**Physical Description:** Cryst. (EtOH aq.)

**Melting Point:** Mp 55-57°

>>Derivative: Oxime

**CAS Registry Number:** 127529-51-5

**Molecular Formula:** C<sub>16</sub>H<sub>17</sub>NO

**Molecular Weight:** 239.316

**Accurate Mass:** 239.131014

**Percentage Composition:** C 80.30%; H 7.16%; N 5.85%; O 6.69%

**Physical Description:** Cryst. (EtOH aq.)

**Melting Point:** Mp 131-132°

**References:**

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 808B, (*nmr*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 1233D, (*ir*)

Cram, D.J. *et al.*, *J.A.C.S.*, 1957, **79**, 2858-2865, (+-form, *synth*)

Bartnik, R. *et al.*, *Bull. Soc. Chim. Fr.*, 1975, 173-177, (*oxime, synth*)