



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

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

CAS Registry Number: 16282-16-9

H3CCH2CHPhCOPh

Molecular Formula: C16H16O

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: C16H16O

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: $[\alpha]_{\text{D}}^{25} +230.2$ (c, 4.99 in C6H6)

>>Variant: (±)-form

CAS Registry Number: 77542-11-1

Molecular Formula: C16H16O

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: C16H17NO

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*)