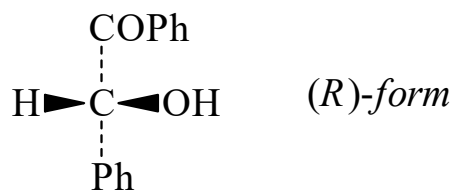




>>Entry Name: Benzoin, 8CI

ENTRY UNDER REVIEW

Synonym(s): 2-Hydroxy-1,2-diphenylethanone, 9CI. α -Hydroxybenzyl phenyl ketone. Benzoylphenylcarbinol. 2-Hydroxy-2-phenylacetophenone. FEMA 2132



CAS Registry Number: 119-53-9

Related CAS Registry Numbers(s): 441-38-3 574-06-1 579-44-2 1459-20-7 8050-35-9 57794-28-2

Molecular Formula: $\text{C}_{14}\text{H}_{12}\text{O}_2$

Molecular Weight: 212.248

Accurate Mass: 212.08373

Percentage Composition: C 79.23%; H 5.70%; O 15.08%

General Statement: For enol form see 1,2-Diphenyl-1,2-ethenediol [DZP29-J](#)

Hazard & Toxicity: LD_{50} (rat, orl) 10,000 mg/kg

Aldrich: 39941-8

Fluka: 12510

>>Variant: (R)-form

CAS Registry Number: 5928-66-5

Molecular Formula: $\text{C}_{14}\text{H}_{12}\text{O}_2$

Molecular Weight: 212.248

Accurate Mass: 212.08373

Percentage Composition: C 79.23%; H 5.70%; O 15.08%

Physical Description: Needles

Melting Point: Mp 131-132.5°

Optical Rotation: $[\alpha]_{\text{D}}^{12} -117.5$ (Me_2CO)

Aldrich: 45994-1

>>Derivative: Ac

CAS Registry Number: 84275-45-6

Molecular Formula: $\text{C}_{16}\text{H}_{14}\text{O}_3$

Molecular Weight: 254.285

Accurate Mass: 254.094295

Percentage Composition: C 75.58%; H 5.55%; O 18.88%

Physical Description: Needles

Optical Rotation: $[\alpha]_{\text{D}}^{14} -217.7$ (CHCl_3)

>>Derivative: Me ether

Synonym(s): 2-Methoxy-1,2-diphenylethanone

CAS Registry Number: 82572-28-9

Molecular Formula: $\text{C}_{15}\text{H}_{14}\text{O}_2$

Molecular Weight: 226.274

Accurate Mass: 226.09938

Percentage Composition: C 79.62%; H 6.24%; O 14.14%

Melting Point: Mp 53-54°

Optical Rotation: $[\alpha]_{\text{D}}^{12} -88.2$ (CHCl_3). $[\alpha]_{\text{D}}^{11} -94.3$ (EtOH)

>>Variant: (S)-form

CAS Registry Number: 5928-67-6

Molecular Formula: $\text{C}_{14}\text{H}_{12}\text{O}_2$

Molecular Weight: 212.248

Accurate Mass: 212.08373

Percentage Composition: C 79.23%; H 5.70%; O 15.08%

Physical Description: Needles

Melting Point: Mp 131-132.5°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +118.4$ (Me_2CO)

Aldrich: 25625-0