



**>>Entry Name: 5-Oxo-5-phenylpentanoic acid**

**Synonym(s):**  $\delta$ -Oxobenzenepentanoic acid, 9Cl. Butyrophenone- $\gamma$ -carboxylic acid. 4-Benzoylbutanoic acid

**CAS Registry Number:** 1501-05-9

PhCOCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>COOH

**Molecular Formula:** C<sub>11</sub>H<sub>12</sub>O<sub>3</sub>

**Molecular Weight:** 192.214

**Accurate Mass:** 192.078645

**Percentage Composition:** C 68.74%; H 6.29%; O 24.97%

**Melting Point:** Mp 127°

**Solubility:** Mod. sol. H<sub>2</sub>O

**Aldrich:** B1268-7

**Fluka:** 12926

**>>Derivative: Oxime**

**Molecular Formula:** C<sub>11</sub>H<sub>13</sub>NO<sub>3</sub>

**Molecular Weight:** 207.229

**Accurate Mass:** 207.089544

**Percentage Composition:** C 63.76%; H 6.32%; N 6.76%; O 23.16%

**Melting Point:** Mp 110°

**>>Derivative: Semicarbazone**

**Melting Point:** Mp 214-215°

**>>Derivative: Me ester**

**CAS Registry Number:** 1501-04-8

**Molecular Formula:** C<sub>12</sub>H<sub>14</sub>O<sub>3</sub>

**Molecular Weight:** 206.241

**Accurate Mass:** 206.094295

**Percentage Composition:** C 69.89%; H 6.84%; O 23.27%

**Physical Description:** Oil

**Melting Point:** Mp -2°

**Boiling Point:** Bp<sub>8</sub> 147-148°

**>>Derivative: Me ester, 2,4-dinitrophenylhydrazone**

**Melting Point:** Mp 149°

**References:**

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 999A, (*nmr*)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 148A, (*ir*)

Yoho, C.W. *et al.*, *J.A.C.S.*, 1952, **74**, 5597, (*synth*)

Le Guillanton, G., *Bull. Soc. Chim. Fr.*, 1969, **82**, 871, (*synth*)

Maurin, J.K. *et al.*, *Acta Cryst. C*, 1994, **50**, 78, (*cryst struct, oxime*)