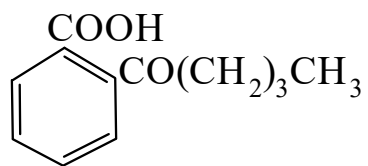




>>Entry Name: 2-(1-Oxopentyl)benzoic acid

Synonym(s): 2-Pentanoylbenzoic acid. **Ligusticumic acid**. Valerophenone-*o*-carboxylic acid



CAS Registry Number: 550-37-8

Molecular Formula: C₁₂H₁₄O₃

Molecular Weight: 206.241

Accurate Mass: 206.094295

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

Boiling Point: Bp_{0.3} 155-165°

>>Derivative: Me ester

Molecular Formula: C₁₃H₁₆O₃

Molecular Weight: 220.268

Accurate Mass: 220.109945

Percentage Composition: C 70.89%; H 7.32%; O 21.79%

Biological Source: Isol. from the fruit of *Ligusticum acutilobum*

Boiling Point: Bp₂ 140-143°

>>Derivative: Amide

Molecular Formula: C₁₂H₁₅NO₂

Molecular Weight: 205.256

Accurate Mass: 205.110279

Percentage Composition: C 70.22%; H 7.37%; N 6.82%; O 15.59%

Melting Point: Mp 136°

References:

Noguchi, T. *et al.*, *Yakugaku Zasshi*, 1936, **56**, 662; *CA*, **31**, 2583

Kariyone, T. *et al.*, *Yakugaku Zasshi*, 1937, **57**, 183; *CA*, **32**, 3361

Watt, D.S., *J.O.C.*, 1974, **39**, 2799, (*synth*)

Naito, T. *et al.*, *Phytochemistry*, 1992, **31**, 1787, (*isol, pmr, cmr*)