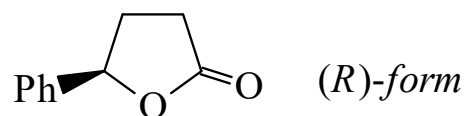




>>Entry Name: Dihydro-5-phenyl-2(3*H*)-furanone, 9CI

Synonym(s): 4-Phenylbutanolide. γ -Phenylbutyrolactone



CAS Registry Number: 1008-76-0

Related CAS Registry Numbers(s): 69814-97-7

Molecular Formula: C₁₀H₁₀O₂

Molecular Weight: 162.188

Accurate Mass: 162.06808

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

Aldrich: 17645-1

>>Variant: (*R*)-form

CAS Registry Number: 111138-03-5

Molecular Formula: C₁₀H₁₀O₂

Molecular Weight: 162.188

Accurate Mass: 162.06808

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

Boiling Point: Bp_{0.1} 99-105°

Optical Rotation: $[\alpha]_D^{25} +35.5$ (c, 2.52 in CHCl₃)

>>Variant: (*S*)-form

CAS Registry Number: 111138-02-4

Molecular Formula: C₁₀H₁₀O₂

Molecular Weight: 162.188

Accurate Mass: 162.06808

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

Physical Description: Solid

Melting Point: Mp 35-36°

Boiling Point: Bp₂ 200°

Optical Rotation: $[\alpha]_D -32.5$ (c, 4.3 in CHCl₃)

>>Variant: ($\pm$)-form

CAS Registry Number: 69814-97-7

Molecular Formula: C₁₀H₁₀O₂

Molecular Weight: 162.188

Accurate Mass: 162.06808

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

Physical Description: Solid

Melting Point: Mp 38°

Boiling Point: Bp₁₁ 171-172°. Bp_{0.6} 115°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 1302C, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 319A, (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1385C, (*ir*)
Cromwell, N.H. *et al.*, *J.A.C.S.*, 1956, **78**, 4412, (*synth*)
Francotte, E. *et al.*, *Helv. Chim. Acta*, 1987, **70**, 1569, (*resoln, abs config*)
Manzocchi, A. *et al.*, *J.C.S. Perkin 1*, 1987, 2753, (*synth, pmr, ms*)
Ballini, R. *et al.*, *Synthesis*, 1987, 711, (*synth, ir, pmr*)
Fukuzawa, S.I. *et al.*, *J.C.S. Perkin 1*, 1988, 1669, (*synth, ir, pmr*)
Barluenga, J. *et al.*, *J.C.S. Perkin 1*, 1988, 3113, (*synth, ir, pmr, cmr, ms*)
Yamamoto, M. *et al.*, *J.O.C.*, 1989, **54**, 1757, (*synth, ir, pmr*)
Nilsson, B.M. *et al.*, *J. Med. Chem.*, 1992, **35**, 285, (*synth*)
Brown, H.C. *et al.*, *J.O.C.*, 1994, **59**, 365, (*R-form*)