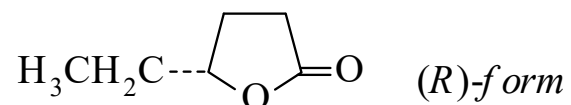




>>Entry Name: 5-Ethylidihydro-2(3*H*)-furanone, 9CI

ENTRY UNDER REVIEW

Synonym(s): 4-Hexanolactone. 4-Caprolactone. 4-Ethylbutyrolactone. 4-Hydroxyhexanoic acid lactone. 4-Hexanolide. γ -Hexalactone. FEMA 2556



CAS Registry Number: 695-06-7

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_2$

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Biological Source: Constit. of soft fruits. Pheromone for the beetle *Trogoderma granarium*

Use/Importance: Used in perfumery

Hazard & Toxicity: Skin irritant

Aldrich: 30383-6

>>Variant: (R)-form

CAS Registry Number: 63357-95-9

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_2$

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Optical Rotation: $[\alpha]_{\text{D}}^{20} +53.2$ (c, 1 in MeOH)

>>Variant: (S)-form

CAS Registry Number: 41035-07-8

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_2$

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Optical Rotation: $[\alpha]_{\text{D}}^{20} -53.2$ (c, 1 in MeOH)

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

CAS Registry Number: 57129-70-1

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_2$

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Use/Importance: Flavouring ingredient

Boiling Point: Bp 215-216°. Bp_{0.2} 50-60° (bath)

Solubility: Sol. aq. alkalis

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1128C, (nmr)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 750C, (ir)

Windaus, A. *et al.*, *Ber.*, 1921, **54**, 586

Meyers, A.I. *et al.*, *J.O.C.*, 1974, **39**, 2783

Sucrow, W. *et al.*, *Chem. Ber.*, 1975, **108**, 48

Ravid, U. *et al.*, *Tetrahedron*, 1978, **34**, 1449

Fuganti, C. *et al.*, *Tet. Lett.*, 1983, **24**, 3753, (synth)

Mori, K. *et al.*, *Tetrahedron*, 1985, **41**, 919, (synth)

Högberg, H.-E. *et al.*, *Acta Chem. Scand., Ser. B*, 1987, **41**, 694, (synth)

Bestmann, H.J. *et al.*, *Tet. Lett.*, 1987, **28**, 2111, (synth)

Yadav, J.S. *et al.*, *Synth. Commun.*, 1989, **19**, 705, (synth)

Núñez, M.T. *et al.*, *J.O.C.*, 1990, **55**, 1928, (synth, pmr, cmr, ms, ir)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1292-1293, (occur, props)

Bertus, P. *et al.*, *Tetrahedron: Asymmetry*, 1999, **10**, 1369-1380, (R-form, synth, pmr, cmr)