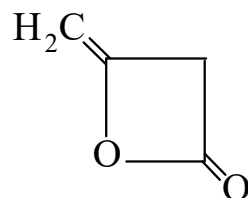




>>Entry Name: 4-Methylene-2-oxetanone, 9CI

Synonym(s): Diketene. Ketene dimer. 3-Hydroxy-3-butenic acid β -lactone



CAS Registry Number: 674-82-8

Molecular Formula: $C_4H_4O_2$

Molecular Weight: 84.074

Accurate Mass: 84.02113

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Use/Importance: Acetylating agent for alcohols and amines

Physical Description: Liq. with pungent odour

Melting Point: Mp -6.5°

Boiling Point: Bp 127.4°

Solubility: Insol. H_2O

Density: d_{20}^{20} 1.09

Refractive Index: n_D^{20} 1.4379

Other Data: Slowly polymerises on standing.

Hazard & Toxicity: Flammable, fl. p. 34° , autoignition temp. 275° . Reacts violently with acids and bases. Eye, skin and respiratory tract irritant. Lachrymator. LD₅₀ (rat, orl) 560 mg/kg

Aldrich: 30205-8

Fluka: 38450

Sigma: D1004

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1124C, (nmr)

Org. Synth., Coll. Vol., 1, 1932, 330, (synth)

Hurd, C.D. *et al.*, *J.A.C.S.*, 1950, **72**, 1461, (struct, synth)

Katz, L. *et al.*, *J.O.C.*, 1952, **17**, 515, (cryst struct)

Johnson, J.R. *et al.*, *J.A.C.S.*, 1953, **75**, 1350, (struct)

Lacey, R.N., *Adv. Org. Chem.*, 1960, **2**, 213, (rev)

Durig, J.R. *et al.*, *Spectrochim. Acta*, 1966, **22**, 1299

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 202

Jarowicki, K. *et al.*, *Chem. Ind. (London)*, 1984, 587, (synth)

Olivares, J.A. *et al.*, *Int. J. Mass Spectrom. Ion Processes*, 1984, **56**, 293, (ms)

Clemens, R.J., *Chem. Rev.*, 1986, **86**, 241, (rev)

Dingwall, J.G. *et al.*, *J.C.S. Perkin 1*, 1986, 2081, (use)

Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 593

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, KFA000

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworths, 1990, 1353

Luxon, S.G., *Hazards in the Chemical Laboratory*, 5th edn., Royal Society of Chemistry, 1992, 485