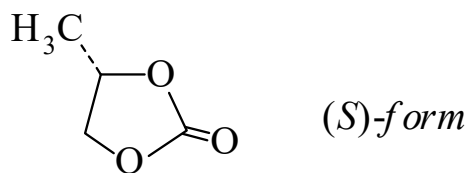




>>Entry Name: 4-Methyl-1,3-dioxolan-2-one, 9CI

Synonym(s): Carbonic acid cyclic propylene ester. Methylethylene carbonate. 1,2-Propylene carbonate



CAS Registry Number: 108-32-7

Molecular Formula: C₄H₆O₃

Molecular Weight: 102.09

Accurate Mass: 102.031695

Percentage Composition: C 47.06%; H 5.92%; O 47.02%

Use/Importance: Much-patented industrial intermed. for polymerisations, etc. Used as an extraction solvent with CHCl₃, low oral acute toxicity. Pharmaceutical excipient (solvent)

Hazard & Toxicity: Fl. p. 135° (oc). Skin and eye irritant

Aldrich: 41422-0

Fluka: 82229

Sigma: P2786

>>Variant: (S)-form

CAS Registry Number: 51260-39-0

Molecular Formula: C₄H₆O₃

Molecular Weight: 102.09

Accurate Mass: 102.031695

Percentage Composition: C 47.06%; H 5.92%; O 47.02%

Boiling Point: Bp₂₅ 100-105°

Optical Rotation: [α]_D²⁵ -1.7 (c, 0.92 in EtOH)

>>Variant: (±)-form

CAS Registry Number: 127128-76-1

Molecular Formula: C₄H₆O₃

Molecular Weight: 102.09

Accurate Mass: 102.031695

Percentage Composition: C 47.06%; H 5.92%; O 47.02%

Physical Description: Liq. with a mild odour

Boiling Point: Bp 240°. Bp_{4.5} 92°. Bp_{0.08} 79-80°

Solubility: Mod. sol. H₂O, CCl₄; misc. Me₂CO, C₆H₆, CHCl₃, Et₂O, EtOH

Density: d₄²⁰ 1.206

Refractive Index: n_D²⁵ 1.4199

Other Data: Dielectric const. ε 64.92, viscosity 2.53 cP

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 613A, (ir)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 932C, (nmr)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 635C, (ir)

Chabrier, P. et al., Bull. Soc. Chim. Fr., 1954, 1142, (synth, props)

Trudell, L.A. et al., Anal. Chim. Acta, 1970, **52**, 343

Jakubiec, R.J. et al., Mikrochim. Acta, 1970, 1199, (use)

Usieli, V. et al., J.O.C., 1974, **39**, 2073, (synth, ir, uv, pmr)

Soga, K. et al., J. Polym. Sci., Polym. Chem. Ed., 1977, **15**, 219, (polym)

J. Am. Coll. Toxicol., 1987, **6**, 23, (props, tox, rev)

Mizuno, T. et al., Synthesis, 1989, 636, (synth, ir, pmr, ms)

Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. et al), American Pharmaceutical Association/Pharmaceutical Press, 1994, 405-406

Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1540

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, CBW500