



Percentage Composition: C 74.19%; H 9.34%; O 16.47%

Use/Importance: Perfumery ingredient

Physical Description: Oil

Boiling Point: Bp 245-246°. Bp₈ 91-92°

>>**Derivative:** Ethylene acetal

Synonym(s): 2-(Phenylmethyl)-1,3-dioxolane, 9CI. 2-Benzyl-1,3-dioxolane

CAS Registry Number: 101-49-5

Molecular Formula: C₁₀H₁₂O₂

Molecular Weight: 164.204

Accurate Mass: 164.08373

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Physical Description: Oil

Boiling Point: Bp₁ 98-99°. Bp₁₂ 115-120°

Density: d₄²⁶ 1.09

Refractive Index: n_D²⁰ 1.5220

Aldrich: 29942-1

Fluka: 13415

>>**Derivative:** Bis(2-methylpropyl) acetal

Synonym(s): [2,2-Bis(2-methylpropoxy)ethyl]benzene, 9CI. FEMA 3384

CAS Registry Number: 68345-22-2

Molecular Formula: C₁₆H₂₆O₂

Molecular Weight: 250.38

Accurate Mass: 250.19328

Percentage Composition: C 76.75%; H 10.47%; O 12.78%

Physical Description: Liq.

Boiling Point: Bp 240°

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 1066C; **2**, 101A, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 230A; 239A, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 998A; 998B; 1279A, (*ir*)
CRC Atlas of Spectral Data and Physical Constants, 937, (*uv, ir, ms*)
Erlenmeyer, E. *et al.*, *Annalen*, 1883, **219**, 179, (*synth*)
Naidan, V.M. *et al.*, *Zh. Org. Khim.*, 1965, **1**, 1377-1383; *J. Org. Chem. USSR (Engl. Transl.)*, 1965, **1**, 1395-1400, (*ethylene acetal, synth, uv*)
Attaway, J.A. *et al.*, *Phytochemistry*, 1966, **5**, 1273, (*isol*)
Hawkes, G.E. *et al.*, *J.O.C.*, 1974, **39**, 1017, (*cmr*)
Pritchard, J.G., *Org. Mass Spectrom.*, 1974, **8**, 103, (*ms*)
Org. Synth., 1974, **54**, 42, (*synth*)
Smith, A.B. *et al.*, *J. Chem. Ecol.*, 1977, **3**, 309
Opdyke, D.L.J., *Food Cosmet. Toxicol.*, 1979, **17**, 377, (*rev, tox*)
Schaefer, T. *et al.*, *Can. J. Chem.*, 1985, **63**, 2597, (*conformn, pmr*)
Lewis, R.J., *Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BBL500
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 657-658
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2177-2181
Katritzky, A.R. *et al.*, *J.O.C.*, 2000, **65**, 1886-1888, (*ethylene acetal, synth, pmr, cmr*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992; PDX000; BEN250