



>>Entry Name: 4-Propyl-1,2-benzenediol, 9CI

ENTRY UNDER REVIEW

Synonym(s): 4-Propylpyrocatechol, 8CI. 4-Propylcatechol

CAS Registry Number: 2525-02-2

Related CAS Registry Numbers(s): 58539-27-8 89266-70-6

Molecular Formula: C₉H₁₂O₂

Molecular Weight: 152.193

Accurate Mass: 152.08373

Percentage Composition: C 71.03%; H 7.95%; O 21.03%

Physical Description: Prisms (C₆H₆)

Melting Point: Mp 60°

Boiling Point: Bp₃₀ 175-180°

>>Derivative: 2-Me ether

Synonym(s): 2-Methoxy-4-propylphenol, 9CI. Cerulignol. Dihydroeugenol. Propylguaiacol. Coerulignol. FEMA 3598

CAS Registry Number: 2785-87-7

Molecular Formula: C₁₀H₁₄O₂

Molecular Weight: 166.219

Accurate Mass: 166.09938

Percentage Composition: C 72.26%; H 8.49%; O 19.25%

Source/Synthesis: Formed by dist. of beechwood

Physical Description: Liq.

Boiling Point: Bp 240-241°. Bp_{0.7} 80-82°

Refractive Index: n_D²⁵ 1.5200

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 2600 mg/kg. LD₅₀ (rbt, skn) 310 mg/kg

Aldrich: W35980-7

>>Derivative: Di-Me ether

Synonym(s): 1,2-Dimethoxy-4-propylbenzene. 4-Propylveratrole

CAS Registry Number: 5888-52-8

Molecular Formula: C₁₁H₁₆O₂

Molecular Weight: 180.246

Accurate Mass: 180.11503

Percentage Composition: C 73.30%; H 8.95%; O 17.75%

Physical Description: Oil

Boiling Point: Bp 247°. Bp₄ 112-114°

References:

Claisen, L. *et al.*, *Annalen*, 1926, **449**, 81-101, (2-Me ether)

Tsukervarik, I.P. *et al.*, *J. Gen. Chem. USSR (Engl. Transl.)*, 1947, **17**, 1009, (synth)

Zbiral, E. *et al.*, *Monatsh. Chem.*, 1961, **92**, 654-666, (synth)

Katritzky, A.R. *et al.*, *Synthesis*, 1994, 499-504, (di-Me ether, synth)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 463, (2-Me ether)

Hu, T.Q. *et al.*, *Can. J. Chem.*, 1997, **75**, 1234-1239, (Me ethers, synth, ir, pmr)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1703-1704, (2-Me ether)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MFM750