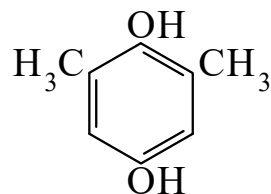




>>Entry Name: 2,6-Dimethyl-1,4-benzenediol, 9CI

Synonym(s): 2,6-Dimethylhydroquinone, 8CI. 2,5-Dihydroxy-*m*-xylene. 2,6-Dimethylquinol. *m*-Xylohydroquinone. 2,6-Xylohydroquinone



CAS Registry Number: 654-42-2

Related CAS Registry Numbers(s): 21111-81-9

Type of Compound Code(s): VG0010

Molecular Formula: C₈H₁₀O₂

Molecular Weight: 138.166

Accurate Mass: 138.06808

Percentage Composition: C 69.55%; H 7.29%; O 23.16%

Biological Source: Claimed isoln. from *Pisum sativum*

Physical Description: Cryst. (xylene)

Melting Point: Mp 149-151°

Other Data: Steam-volatile. Isoln. as nat. prod. unconfirmed

Hazard & Toxicity: Human and exp. reprod. effects (reduced fertility). Exp. teratogenic effects. LD₅₀ (mus, orl) 186 mg/kg

>>Derivative: 1-Me ether

Synonym(s): 4-Methoxy-3,5-dimethylphenol

Molecular Formula: C₉H₁₂O₂

Molecular Weight: 152.193

Accurate Mass: 152.08373

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

Physical Description: Plates

Melting Point: Mp 84-85°

Other Data: Incorrectly named as "2,6-dimethyl-4-methoxyphenol" and incorrect formula of C₉H₁₄O₃ given

>>Derivative: 4-Me ether

Synonym(s): 4-Methoxy-2,6-dimethylphenol

CAS Registry Number: 2431-91-6

Molecular Formula: C₉H₁₂O₂

Molecular Weight: 152.193

Accurate Mass: 152.08373

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

Physical Description: Needles (petrol)

Melting Point: Mp 77°

pKa Value: pK_{a1} 10.84 (25°)

>>Derivative: Di-Me ether

Synonym(s): 1,4-Dimethoxy-2,6-dimethylbenzene

Molecular Formula: C₁₀H₁₄O₂

Molecular Weight: 166.219

Accurate Mass: 166.09938

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

Physical Description: Oil

References:

Bamberger, E. *et al.*, *Annalen*, 1901, **316**, 302, (*synth*)

Bruice, T.C. *et al.*, *J.O.C.*, 1953, **18**, 83, (*1-Me ether*)

Nilsson, J.L.G. *et al.*, *Acta Pharm. Suec.*, 1968, **5**, 215; *CA*, **69**, 106132, (*synth*)

Carpino, L.A. *et al.*, *J.O.C.*, 1989, **54**, 3303, (*synth, pmr*)

Elix, J.A. *et al.*, *Aust. J. Chem.*, 1993, **46**, 95, (*di-Me ether*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DSG700

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