



>>Entry Name: 4-(1-Methylethenyl)phenol, 9CI

Synonym(s): 4-Isopropenylphenol. *p*-Hydroxy- α -methylstyrene. 2-(4-Hydroxyphenyl)propene

CAS Registry Number: 4286-23-1

Molecular Formula: C₉H₁₀O

Molecular Weight: 134.177

Accurate Mass: 134.073165

Percentage Composition: C 80.56%; H 7.51%; O 11.92%

Physical Description: Cryst. (C₆H₆/hexane or 1,2-dichloroethane)

Melting Point: Mp 85-86° (74-75°)

>>Derivative: Ac

CAS Registry Number: 2759-56-0

Molecular Formula: C₁₁H₁₂O₂

Molecular Weight: 176.215

Accurate Mass: 176.08373

Percentage Composition: C 74.98%; H 6.86%; O 18.16%

Physical Description: Liq.

Boiling Point: Bp_{0.3} 83-85°

>>Derivative: Benzoyl

CAS Registry Number: 72537-29-2

Molecular Formula: C₁₆H₁₄O₂

Molecular Weight: 238.285

Accurate Mass: 238.09938

Percentage Composition: C 80.65%; H 5.92%; O 13.43%

Physical Description: Needles (EtOH)

Melting Point: Mp 112-113.5°

>>Derivative: Me ether

Synonym(s): 1-Methoxy-4-(1-methylethenyl)benzene, 9CI. 4-Isopropenylanisole. *p*-Methoxy- α -methylstyrene. 2-(4-Methoxyphenyl)propene

CAS Registry Number: 1712-69-2

Molecular Formula: C₁₀H₁₂O

Molecular Weight: 148.204

Accurate Mass: 148.088815

Percentage Composition: C 81.04%; H 8.16%; O 10.80%

Physical Description: Cryst.

Melting Point: Mp 34°

Boiling Point: Bp₂ 90°

References:

- Seymour, D. *et al.*, *J.A.C.S.*, 1948, **70**, 1177-1179, (*Me ether*)
Dale, W.J. *et al.*, *J.A.C.S.*, 1956, **78**, 2543, (*benzoyl*)
Corson, B.B. *et al.*, *J.O.C.*, 1958, **23**, 544-549, (*synth*)
Kahovec, J. *et al.*, *Coll. Czech. Chem. Comm.*, 1971, **36**, 1986-1993, (*synth, pmr*)
Padgett, S.R. *et al.*, *Biochemistry*, 1985, **24**, 5826-5839, (*synth, Ac, pmr*)
Dai, S.H. *et al.*, *J.O.C.*, 1985, **50**, 1722-1725, (*synth, pmr*)
Friebolin, H. *et al.*, *Liebigs Ann./Recl.*, 1997, 385-390, (*Me ether*)
Shukla, D. *et al.*, *J.O.C.*, 2000, **65**, 6167-6172, (*Me ether, synth, pmr, cmr, ms*)