



>>Entry Name: 2-Hydroxy-3-isopropyl-6-methylbenzoic acid

Synonym(s): 2-Hydroxy-6-methyl-3-(1-methylethyl)benzoic acid, 9Cl. 3-Hydroxy-*p*-cymene-2-carboxylic acid, 8Cl. 3-Isopropyl-6-methylsalicylic acid. 6-Hydroxy-5-isopropyl-*o*-toluic acid. *o*-Thymotinic acid. Thymol-2-carboxylic acid

CAS Registry Number: 548-51-6

Molecular Formula: C₁₁H₁₄O₃

Molecular Weight: 194.23

Accurate Mass: 194.094295

Percentage Composition: C 68.02%; H 7.26%; O 24.71%

Use/Importance: Bactericidal

Physical Description: Needles (H₂O, C₆H₆ or petrol)

Melting Point: Mp 127°

Other Data: Steam-volatile

Aldrich: 33991-1

>>Derivative: Me ester

CAS Registry Number: 6547-90-6

Molecular Formula: C₁₂H₁₆O₃

Molecular Weight: 208.257

Accurate Mass: 208.109945

Percentage Composition: C 69.21%; H 7.74%; O 23.05%

Physical Description: Yellow oil

Boiling Point: Bp_{18.5} 142°

>>Derivative: Me ether

Synonym(s): 3-Isopropyl-2-methoxy-6-methylbenzoic acid

CAS Registry Number: 72135-27-4

Molecular Formula: C₁₂H₁₆O₃

Molecular Weight: 208.257

Accurate Mass: 208.109945

Percentage Composition: C 69.21%; H 7.74%; O 23.05%

Physical Description: Cryst. (petrol)

Melting Point: Mp 83-84°

Boiling Point: Bp_{0.15} 148-150°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1143B, (*nmr*)

Spallino, R. *et al.*, *Gazz. Chim. Ital.*, 1909, **39**, 325

Royer, R. *et al.*, *Bull. Soc. Chim. Fr.*, 1955, 1421