



>>Entry Name: 3-Methyl-2-benzofurancarboxylic acid, 9CI

Synonym(s): 3-Methylcoumarilic acid. 3-Methylcoumarone-2-carboxylic acid

CAS Registry Number: 24673-56-1

Molecular Formula: C₁₀H₈O₃

Molecular Weight: 176.171

Accurate Mass: 176.047345

Percentage Composition: C 68.18%; H 4.58%; O 27.25%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 192-194°

>>Derivative: Me ester

Molecular Formula: C₁₁H₁₀O₃

Molecular Weight: 190.198

Accurate Mass: 190.062995

Percentage Composition: C 69.46%; H 5.30%; O 25.24%

Physical Description: Needles (H₂O)

Melting Point: Mp 70°

>>Derivative: Et ester

CAS Registry Number: 22367-82-4

Molecular Formula: C₁₂H₁₂O₃

Molecular Weight: 204.225

Accurate Mass: 204.078645

Percentage Composition: C 70.58%; H 5.92%; O 23.50%

Physical Description: Plates (C₆H₆)

Melting Point: Mp 51°

Boiling Point: Bp₁₇ 170°

References:

Org. Synth., Coll. Vol., 4, 1963, 590, (*synth*)

Sila, B., *Pol. J. Chem. (Rocz. Chem.)*, 1969, **43**, 1413, (*synth*)

Topolski, M. *et al.*, *J.O.C.*, 1995, **60**, 5588, (*synth, pmr*)

Bedford, S.B. *et al.*, *J.C.S. Perkin 1*, 1996, 2827, (*synth, Et ester, ir, pmr*)