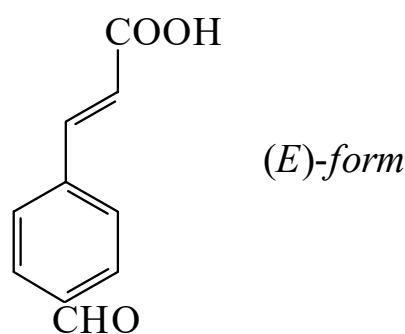




>>Entry Name: 3-(4-Formylphenyl)-2-propenoic acid, 9CI

Synonym(s): *p*-Formylcinnamic acid



CAS Registry Number: 23359-08-2

Molecular Formula: C₁₀H₈O₃

Molecular Weight: 176.171

Accurate Mass: 176.047345

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

Aldrich: 17876-4

>>Variant: (*E*)-form

CAS Registry Number: 66885-68-5

Molecular Formula: C₁₀H₈O₃

Molecular Weight: 176.171

Accurate Mass: 176.047345

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

Physical Description: Prisms (EtOH)

Melting Point: Mp 250° (247-249°)

Other Data: A cryst. struct. detn. carried out in 1985 was erroneously reported

>>Derivative: Me ester

CAS Registry Number: 58045-41-3

Molecular Formula: C₁₁H₁₀O₃

Molecular Weight: 190.198

Accurate Mass: 190.062995

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

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 82-83° (79-82°)

>>Variant: (*Z*)-form

CAS Registry Number: 81509-16-2

Molecular Formula: C₁₀H₈O₃

Molecular Weight: 176.171

Accurate Mass: 176.047345

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

>>Derivative: Me ester

CAS Registry Number: 71093-79-3

Molecular Formula: C₁₁H₁₀O₃

Molecular Weight: 190.198

Accurate Mass: 190.062995

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

Other Data: No phys. props. reported

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1052C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 182B, (*ir*)

Low, W., *Annalen*, 1885, **231**, 361, (*synth*)

Ephraim, F., *Ber.*, 1901, **34**, 2784, (*synth, Me ester*)

Wiley, R.H. *et al.*, *J.A.C.S.*, 1949, **71**, 2429, (*synth*)

Castells, J. *et al.*, *J.C.S. Perkin 1*, 1979, **1**, (*synth, pmr, isom*)

Ichimura, K. *et al.*, *J. Polym. Sci., Part A: Polym. Chem.*, 1987, **25**, 1579, (*synth, use*)

Nakanish, H. *et al.*, *Acta Cryst. C*, 1989, **45**, 1753

Harris, K.D.M. *et al.*, *J.C.S. Perkin 2*, 1994, 1201, (*cryst struct*)