



>>Entry Name: 3-(4-Nitrophenyl)-1-phenyl-2-propen-1-one, 9CI

Synonym(s): 4-Nitrochalcone, 8CI

CAS Registry Number: 1222-98-6

Molecular Formula: C₁₅H₁₁NO₃

Molecular Weight: 253.257

Accurate Mass: 253.073894

Percentage Composition: C 71.14%; H 4.38%; N 5.53%; O 18.95%

Aldrich: 15748-1

>>Variant: (E)-form

CAS Registry Number: 20432-02-4

Molecular Formula: C₁₅H₁₁NO₃

Molecular Weight: 253.257

Accurate Mass: 253.073894

Percentage Composition: C 71.14%; H 4.38%; N 5.53%; O 18.95%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 164°

>>Variant: (Z)-form

Molecular Formula: C₁₅H₁₁NO₃

Molecular Weight: 253.257

Accurate Mass: 253.073894

Percentage Composition: C 71.14%; H 4.38%; N 5.53%; O 18.95%

Physical Description: Cryst. (C₆H₆/hexane)

Melting Point: Mp 97°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 53A, (*ir*)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 56A, (*pmr*)

Davey, W. *et al.*, *J.C.S.*, 1957, 1008, (*synth*)

Noyce, D.S. *et al.*, *J.A.C.S.*, 1961, **83**, 2525, (*synth*)