



>>Entry Name: **3-(4-Nitrophenyl)-2-propenal**, 9CI

Synonym(s): *p*-Nitrocinnamaldehyde, 8CI. 3-*p*-Nitrophenylacrolein

CAS Registry Number: 1734-79-8

Related CAS Registry Numbers(s): 40413-03-4

Molecular Formula: C₉H₇NO₃

Molecular Weight: 177.159

Accurate Mass: 177.042594

Percentage Composition: C 61.02%; H 3.98%; N 7.91%; O 27.09%

Physical Description: Needles (EtOH or H₂O)

Melting Point: Mp 141-142°

Aldrich: 28167-0

Fluka: 74115

>>Derivative: (*E*)-Oxime

CAS Registry Number: 40413-04-5

Molecular Formula: C₉H₈N₂O₃

Molecular Weight: 192.174

Accurate Mass: 192.053493

Percentage Composition: C 56.25%; H 4.20%; N 14.58%; O 24.98%

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 158°

>>Derivative: (*E*)-Oxime, *O*-Ac

Molecular Formula: C₁₁H₁₀N₂O₄

Molecular Weight: 234.211

Accurate Mass: 234.064058

Percentage Composition: C 56.41%; H 4.30%; N 11.96%; O 27.32%

Physical Description: Yellow cryst.

Melting Point: Mp 158°

>>Derivative: Phenylhydrazone

Physical Description: Orange-red cryst. (EtOH)

Melting Point: Mp 180-181°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 930C, (*nmr*)

Grammaticakis, P., *C. R. Hebd. Seances Acad. Sci.*, 1954, **239**, 883, (*uv*)

Savin, V.I. *et al.*, *J. Org. Chem. USSR (Engl. Transl.)*, 1973, **6**, 1130, (*ir*)

Meyers, A.I. *et al.*, *J.O.C.*, 1973, **38**, 36, (*synth*)

Cresp, T.M. *et al.*, *J.C.S. Perkin I*, 1974, 37, (*synth*)

Savin, V.I. *et al.*, *J. Org. Chem. USSR (Engl. Transl.)*, 1975, **11**, 1157, (*pmr*)

Bellassoued, M. *et al.*, *J.O.C.*, 1993, **58**, 2517, (*synth, pmr, ir*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, NFT425