



>>Entry Name: **1-(4-Nitrophenyl)-2-phenylethylene**

Synonym(s): 1-Nitro-4-(2-phenethenyl)benzene, 9CI. 4-Nitrostilbene. 1-Nitro-4-styrylbenzene

CAS Registry Number: 4003-94-5

Molecular Formula: C₁₄H₁₁NO₂

Molecular Weight: 225.246

Accurate Mass: 225.078979

Percentage Composition: C 74.65%; H 4.92%; N 6.22%; O 14.21%

Hazard & Toxicity: Poss. carcinogen (equivocal data)

Rare Chemicals Library: S91420-7

>>Variant: (*E*)-form

CAS Registry Number: 1694-20-8

Molecular Formula: C₁₄H₁₁NO₂

Molecular Weight: 225.246

Accurate Mass: 225.078979

Percentage Composition: C 74.65%; H 4.92%; N 6.22%; O 14.21%

Physical Description: Pale-yellow needles (EtOH)

Melting Point: Mp 155°

Boiling Point: Bp₉ 170°

>>Variant: (*Z*)-form

CAS Registry Number: 6624-53-9

Molecular Formula: C₁₄H₁₁NO₂

Molecular Weight: 225.246

Accurate Mass: 225.078979

Percentage Composition: C 74.65%; H 4.92%; N 6.22%; O 14.21%

Physical Description: Brownish-yellow plates (EtOH)

Melting Point: Mp 65°

References:

Gueslan, H. *et al.*, *Tetrahedron*, 1967, **23**, 187, (*nmr*)

Itier, J. *et al.*, *Bull. Soc. Chim. Fr.*, 1969, 3528, (*uv*)

Exner, O. *et al.*, *Coll. Czech. Chem. Comm.*, 1972, **37**, 2156, (*ir*)

Doucet, J.P. *et al.*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1972, **69**, 188, (*nmr*)

Bakke, J.M., *Acta Chem. Scand., Ser. B*, 1979, **29**, 667, (*synth*)

Colas, C. *et al.*, *Eur. J. Org. Chem.*, 1999, 1357-1366, (*synth, pmr, cmr, ms*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, NMC000