



>>Entry Name: 3-(4,5-Dihydroxy-2-nitrophenyl)-2-propenoic acid, 9CI
Synonym(s): 4,5-Dihydroxy-2-nitrocinnamic acid, 8CI. 6-Nitrocaffeic acid

Related CAS Registry Numbers(s): 58749-45-4

Molecular Formula: C₉H₇NO₆

Molecular Weight: 225.157

Accurate Mass: 225.027339

Percentage Composition: C 48.01%; H 3.13%; N 6.22%; O 42.64%

>>Derivative: Di-Me ether

CAS Registry Number: 20567-38-8

Molecular Formula: C₁₁H₁₁NO₆

Molecular Weight: 253.211

Accurate Mass: 253.058639

Percentage Composition: C 52.18%; H 4.38%; N 5.53%; O 37.91%

Physical Description: Yellow cryst. (AcOH)

Melting Point: Mp 292°

Aldrich: 34599-7

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1060C, (*nmr*)

Kefford, J.F., *J.C.S.*, 1940, 1209

Schofield, K. *et al.*, *J.C.S.*, 1945, 519, (*synth*)