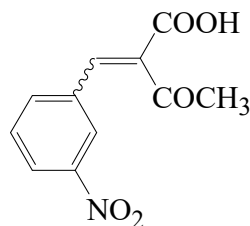




>>Entry Name: 2-(3-Nitrobenzylidene)-3-oxobutanoic acid

Synonym(s): 2-[(3-Nitrophenyl)methylene]-3-oxobutanoic acid, 9Cl. 2-(3-Nitrobenzylidene)acetoacetic acid



CAS Registry Number: 101072-61-1

Molecular Formula: C₁₁H₉NO₅

Molecular Weight: 235.196

Accurate Mass: 235.048074

Percentage Composition: C 56.17%; H 3.86%; N 5.96%; O 34.01%

Use/Importance: Esters are intermediates in the Hantzsch synthesis of 1,4-dihydropyridines related to Nitrendipine [FLZ33-G](#)

Physical Description: Dark yellow cryst. (2-propanol)

Melting Point: Mp 167-170°

>>Derivative: Me ester

CAS Registry Number: 39562-17-9

Extra CAS Registry Numbers(s): 118431-03-1 119128-13-1

Molecular Formula: C₁₂H₁₁NO₅

Molecular Weight: 249.223

Accurate Mass: 249.063724

Percentage Composition: C 57.83%; H 4.45%; N 5.62%; O 32.10%

Melting Point: Mp 158°

>>Derivative: Et ester

CAS Registry Number: 39562-16-8

Molecular Formula: C₁₃H₁₃NO₅

Molecular Weight: 263.249

Accurate Mass: 263.079374

Percentage Composition: C 59.31%; H 4.98%; N 5.32%; O 30.39%

Melting Point: Mp 107°

>>Derivative: Isopropyl ester

CAS Registry Number: 39562-25-9

Molecular Formula: C₁₄H₁₅NO₅

Molecular Weight: 277.276

Accurate Mass: 277.095024

Percentage Composition: C 60.64%; H 5.45%; N 5.05%; O 28.85%

Melting Point: Mp 94°

References:

Meyer, H. *et al.*, *Arzneim.-Forsch.*, 1981, **31**, 407-409, (*esters, synth*)

Biswas, C.J. *et al.*, *Biochem. Biophys. Res. Commun.*, 1986, **134**, 922-927, (*synth*)