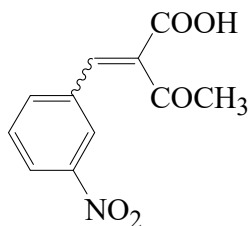




**>>Entry Name: 2-(3-Nitrobenzylidene)-3-oxobutanoic acid**

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



**CAS Registry Number:** 101072-61-1

**Molecular Formula:** C<sub>11</sub>H<sub>9</sub>NO<sub>5</sub>

**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:** C<sub>12</sub>H<sub>11</sub>NO<sub>5</sub>

**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:** C<sub>13</sub>H<sub>13</sub>NO<sub>5</sub>

**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:** C<sub>14</sub>H<sub>15</sub>NO<sub>5</sub>

**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*)