



>>Entry Name: 3-Oxoheptanedioic acid, 9CI

CAS Registry Number: 1608-78-2

HOOCCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>COCH<sub>2</sub>COOH

Molecular Formula: C<sub>7</sub>H<sub>10</sub>O<sub>5</sub>

Molecular Weight: 174.153

Accurate Mass: 174.052825

Percentage Composition: C 48.28%; H 5.79%; O 45.93%

Melting Point: Mp 70-75 dec.°

>>Derivative: Di-Me ester

CAS Registry Number: 15890-00-3

Molecular Formula: C<sub>9</sub>H<sub>14</sub>O<sub>5</sub>

Molecular Weight: 202.207

Accurate Mass: 202.084125

Percentage Composition: C 53.46%; H 6.98%; O 39.56%

Boiling Point: Bp<sub>0.5</sub> 120°

>>Derivative: Diethyl ester

CAS Registry Number: 40420-22-2

Molecular Formula: C<sub>11</sub>H<sub>18</sub>O<sub>5</sub>

Molecular Weight: 230.26

Accurate Mass: 230.115425

Percentage Composition: C 57.38%; H 7.88%; O 34.74%

Boiling Point: Bp<sub>0.5</sub> 130-132°

Aldrich: 23248-3

Fluka: 75943

#### References:

*Aldrich Library of NMR Spectra*, 2nd edn., 1983, **1**, 583A

Birkofer, L. *et al.*, *Chem. Ber.*, 1953, **86**, 32, (*synth*)

Thoma, H. *et al.*, *Annalen*, 1983, 1237, (*synth, ir, pmr*)

Celerier, J.P. *et al.*, *J. Het. Chem.*, 1988, **25**, 1275, (*synth, ir*)

Schmidt, H.W. *et al.*, *Org. Prep. Proced. Int.*, 1988, **20**, 184, (*synth*)