



>>Entry Name: **3,3-Dimethyl-2-oxobutanoic acid**, 9CI

Synonym(s): 3,3-Dimethyl-2-oxobutyric acid, 8CI. Trimethylpyruvic acid. *tert*-Butylglyoxylic acid. 2-Oxo-*tert*-butylacetic acid

CAS Registry Number: 815-17-8

(H₃C)₃CCOCOOH

Molecular Formula: C₆H₁₀O₃

Molecular Weight: 130.143

Accurate Mass: 130.062995

Percentage Composition: C 55.37%; H 7.74%; O 36.88%

Physical Description: Needles (Et₂O)

Melting Point: Mp 90-91°

Boiling Point: Bp₁₅ 80°

Solubility: Spar. sol. H₂O, sol. Et₂O

Rare Chemicals Library: S87619-4

>>Derivative: Me ester

CAS Registry Number: 38941-46-7

Molecular Formula: C₇H₁₂O₃

Molecular Weight: 144.17

Accurate Mass: 144.078645

Percentage Composition: C 58.32%; H 8.39%; O 33.29%

Boiling Point: Bp 160-162°. Bp₂₀ 69-70°

>>Derivative: Me ester, oxime

Molecular Formula: C₇H₁₃NO₃

Molecular Weight: 159.185

Accurate Mass: 159.089544

Percentage Composition: C 52.82%; H 8.23%; N 8.80%; O 30.15%

Physical Description: Cryst. (Et₂O/petrol)

Melting Point: Mp 66°

>>Derivative: Me ester, semicarbazone

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 125°

>>Derivative: Oxime

Molecular Formula: C₆H₁₁NO₃

Molecular Weight: 145.158

Accurate Mass: 145.073894

Percentage Composition: C 49.65%; H 7.64%; N 9.65%; O 33.07%

Physical Description: Leaflets + H₂O (EtOH)

Melting Point: Mp 85-86° (anhyd. 121°)

>>Derivative: Semicarbazone

Physical Description: Cryst. (H₂O)

Melting Point: Mp 195°

References:

Rabjohn, N. *et al.*, *J.O.C.*, 1970, **35**, 3726, (*synth*)

Jaeger, D.A. *et al.*, *J.A.C.S.*, 1979, **101**, 717, (*synth*, *ir*, *pmr*)