



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

Synonym(s): *tert*-Butylacetic acid

CAS Registry Number: 1070-83-3

(H₃C)₃CCH₂COOH

Molecular Formula: C₆H₁₂O₂

Molecular Weight: 116.16

Accurate Mass: 116.08373

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Physical Description: Liq.

Melting Point: Mp 6-7°

Boiling Point: Bp 190°

Density: d₄²⁵ 0.908

pKa Value: pK_a 6.37 (25°, EtOH aq.)

Refractive Index: n_D²⁵ 1.4083

Aldrich: B8840-3

Fluka: 39850

>>Derivative: Me ester

CAS Registry Number: 10250-48-3

Molecular Formula: C₇H₁₄O₂

Molecular Weight: 130.186

Accurate Mass: 130.09938

Percentage Composition: C 64.58%; H 10.84%; O 24.58%

Boiling Point: Bp 126°

Rare Chemicals Library: S88459-6

>>Derivative: Chloride

CAS Registry Number: 7065-46-5

Molecular Formula: C₆H₁₁ClO

Molecular Weight: 134.605

Accurate Mass: 134.049842

Percentage Composition: C 53.54%; H 8.24%; Cl 26.34%; O 11.89%

Melting Point: Mp 127-129°

Refractive Index: n_D²⁰ 1.4210

Aldrich: B8880-2

Fluka: 19405

>>Derivative: Amide

Molecular Formula: C₆H₁₃NO

Molecular Weight: 115.175

Accurate Mass: 115.099714

Percentage Composition: C 62.57%; H 11.38%; N 12.16%; O 13.89%

Physical Description: Leaflets

Melting Point: Mp 132°

>>Derivative: Anilide

Molecular Formula: C₁₂H₁₇NO

Molecular Weight: 191.272

Accurate Mass: 191.131014

Percentage Composition: C 75.35%; H 8.96%; N 7.32%; O 8.36%

Melting Point: Mp 132°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 761B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 488D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 579B; 770A, (*ir*)

Gryszkiewicz-Trochimowski, E. *et al.*, *Bull. Soc. Chim. Fr.*, 1951, 269, (*synth*)

Bott, K., *Chem. Ber.*, 1967, **100**, 978, (*synth*)