



>>Entry Name: 2,2-Dimethylhexanoic acid, 9CI

CAS Registry Number: 813-72-9

$\text{H}_3\text{C}(\text{CH}_2)_3\text{C}(\text{CH}_3)_2\text{COOH}$

Molecular Formula: $\text{C}_8\text{H}_{16}\text{O}_2$

Molecular Weight: 144.213

Accurate Mass: 144.11503

Percentage Composition: C 66.63%; H 11.18%; O 22.19%

Boiling Point: Bp₇₂₆ 216-220°. Bp₁₅ 115-117°

>>Derivative: Me ester

CAS Registry Number: 813-69-4

Molecular Formula: $\text{C}_9\text{H}_{18}\text{O}_2$

Molecular Weight: 158.24

Accurate Mass: 158.13068

Percentage Composition: C 68.31%; H 11.46%; O 20.22%

Boiling Point: Bp 168.5-170°

>>Derivative: Et ester

CAS Registry Number: 38068-09-6

Molecular Formula: $\text{C}_{10}\text{H}_{20}\text{O}_2$

Molecular Weight: 172.267

Accurate Mass: 172.14633

Percentage Composition: C 69.72%; H 11.70%; O 18.58%

Boiling Point: Bp 181-182.5°

>>Derivative: Chloride

CAS Registry Number: 17701-31-4

Molecular Formula: $\text{C}_8\text{H}_{15}\text{ClO}$

Molecular Weight: 162.659

Accurate Mass: 162.081142

Percentage Composition: C 59.07%; H 9.29%; Cl 21.80%; O 9.84%

Boiling Point: Bp₁₀ 55°

>>Derivative: Amide

CAS Registry Number: 20923-67-5

Molecular Formula: $\text{C}_8\text{H}_{17}\text{NO}$

Molecular Weight: 143.228

Accurate Mass: 143.131014

Percentage Composition: C 67.09%; H 11.96%; N 9.78%; O 11.17%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 92-92.5°

>>Derivative: Nitrile

Synonym(s): 2-Cyano-2-methylhexane

CAS Registry Number: 55897-65-9

Molecular Formula: $\text{C}_8\text{H}_{15}\text{N}$

Molecular Weight: 125.213

Accurate Mass: 125.120449

Percentage Composition: C 76.74%; H 12.07%; N 11.19%

Boiling Point: Bp 171°

References:

McElvain, S.M. *et al.*, *J.A.C.S.*, 1953, **75**, 3987-3993, (*synth*)

Murayama, M. *et al.*, *Pharm. Bull.*, 1958, **6**, 186-194, (*synth*)

Le Borgine, J.F. *et al.*, *Synthesis*, 1976, 238-240, (*nitrile, synth, ir*)

Dostovalova, V.I. *et al.*, *Org. Magn. Reson.*, 1983, **21**, 11-19, (*cmr*)

Takahashi, Y. *et al.*, *Synth. Commun.*, 1989, **19**, 1945-1954, (*synth*)