



>>Entry Name: 11-Methyldodecanoic acid, 9CI

Synonym(s): Isotridecanoic acid

CAS Registry Number: 5681-98-1

$(\text{H}_3\text{C})_2\text{CH}(\text{CH}_2)_9\text{COOH}$

Molecular Formula: $\text{C}_{13}\text{H}_{26}\text{O}_2$

Molecular Weight: 214.347

Accurate Mass: 214.19328

Percentage Composition: C 72.85%; H 12.23%; O 14.93%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 37-40°

Boiling Point: Bp₁₆ 189-190°

Refractive Index: n_D⁶⁰ 1.4293

>>Derivative: Et ester

Molecular Formula: $\text{C}_{15}\text{H}_{30}\text{O}_2$

Molecular Weight: 242.401

Accurate Mass: 242.22458

Percentage Composition: C 74.33%; H 12.47%; O 13.20%

Boiling Point: Bp₁₀ 155°

>>Derivative: Chloride

Molecular Formula: $\text{C}_{13}\text{H}_{25}\text{ClO}$

Molecular Weight: 232.793

Accurate Mass: 232.159392

Percentage Composition: C 67.07%; H 10.82%; Cl 15.23%; O 6.87%

Physical Description: Oil

Boiling Point: Bp₁₈ 156-157°

>>Derivative: Amide

Molecular Formula: $\text{C}_{13}\text{H}_{27}\text{NO}$

Molecular Weight: 213.362

Accurate Mass: 213.209264

Percentage Composition: C 73.18%; H 12.75%; N 6.56%; O 7.50%

Physical Description: Needles (MeOH)

Melting Point: Mp 103°

References:

Sy, M. *et al.*, *C. R. Hebd. Seances Acad. Sci.*, 1954, **239**, 1813-1815, (*synth, derivs*)

Shortland, F.B. *et al.*, *Biochem. J.*, 1955, **61**, 702-704, (*synth*)

Dhar, M.L. *et al.*, *J.C.S.*, 1964, 842-861, (*synth*)

Lewis, R.N.A.H. *et al.*, *Biochem. J.*, 1985, **24**, 2431-2439, (*synth*)