



>>Entry Name: 8-Methylnonanoic acid, 9CI

CAS Registry Number: 5963-14-4

$(\text{H}_3\text{C})_2\text{CH}(\text{CH}_2)_6\text{COOH}$

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%

Use/Importance: Intermed. in synth of [LBD66-I](#)

Physical Description: Cryst. (H_2O)

Melting Point: Mp 22.5-24°

Boiling Point: Bp_{0.3} 93-95°

>>Derivative: Me ester

CAS Registry Number: 5129-54-4

Molecular Formula: $\text{C}_{11}\text{H}_{22}\text{O}_2$

Molecular Weight: 186.294

Accurate Mass: 186.16198

Percentage Composition: C 70.92%; H 11.90%; O 17.18%

Boiling Point: Bp₁₀ 92-95°

>>Derivative: Amide

CAS Registry Number: 3085-26-5

Molecular Formula: $\text{C}_{10}\text{H}_{21}\text{NO}$

Molecular Weight: 171.282

Accurate Mass: 171.162314

Percentage Composition: C 70.12%; H 12.36%; N 8.18%; O 9.34%

Melting Point: Mp 103.5-104.5°

References:

Fieser, L.F. *et al.*, *J.A.C.S.*, 1948, **70**, 3174-3180, (*synth*)

Hougen, F.W. *et al.*, *J.C.S.*, 1953, 98-102, (*synth*)

Milburn, A.H. *et al.*, *J.C.S.*, 1954, 3344-3351, (*synth*)

Ackroyd, J. *et al.*, *J. Chem. Res., Synop.*, 1987, 344-345, (*synth*)

Kaga, H. *et al.*, *Synthesis*, 1989, 864-866, (*synth, ir, pmr, ms*)

Hassarajani, S.A. *et al.*, *Indian J. Chem., Sect. B*, 1995, **34**, 429-431, (*Me ester, synth, ir, pmr*)