



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

ENTRY UNDER REVIEW

Synonym(s): 1-Heptyne-1-carboxylic acid

CAS Registry Number: 5663-96-7

$\text{H}_3\text{C}(\text{CH}_2)_4\text{C}\equiv\text{CCOOH}$

Molecular Formula: $\text{C}_8\text{H}_{12}\text{O}_2$

Molecular Weight: 140.182

Accurate Mass: 140.08373

Percentage Composition: C 68.55%; H 8.63%; O 22.83%

Use/Importance: Fungicide

Physical Description: Liq.

Melting Point: Fp 2-5°

Boiling Point: Bp 180-220° dec.. Bp₁₉ 148-149°

Density: d_4^{13} 0.962

Refractive Index: n_D^{20} 1.4595

Aldrich: 24386-8

Rare Chemicals Library: S37016-9

Sigma: O8505

>>Derivative: Me ester

Synonym(s): Methyl 2-octynoate. Methyl heptyne carbonate. FEMA 2729

CAS Registry Number: 111-12-6

Molecular Formula: $\text{C}_9\text{H}_{14}\text{O}_2$

Molecular Weight: 154.208

Accurate Mass: 154.09938

Percentage Composition: C 70.10%; H 9.15%; O 20.75%

Use/Importance: Perfumery ingredient

Physical Description: Liq. with violet odour

Boiling Point: Bp₂₀ 107°. Bp₁₀ 94°

Refractive Index: n_D^{20} 1.4464

Aldrich: 27750-9

Fluka: 74975

Rare Chemicals Library: S35318-3

>>Derivative: Et ester

CAS Registry Number: 10519-20-7

Molecular Formula: $\text{C}_{10}\text{H}_{16}\text{O}_2$

Molecular Weight: 168.235

Accurate Mass: 168.11503

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Boiling Point: Bp_{0.2} 51-52°

Rare Chemicals Library: S41410-7

>>Derivative: Chloride

Molecular Formula: $\text{C}_8\text{H}_{11}\text{ClO}$

Molecular Weight: 158.627

Accurate Mass: 158.049842

Percentage Composition: C 60.57%; H 6.99%; Cl 22.35%; O 10.09%

Boiling Point: Bp₁₇ 88-90°

>>Derivative: Amide

Molecular Formula: $\text{C}_8\text{H}_{13}\text{NO}$

Molecular Weight: 139.197

Accurate Mass: 139.099714

Percentage Composition: C 69.03%; H 9.41%; N 10.06%; O 11.49%

Physical Description: Plates (EtOH)

Melting Point: Mp 91°