



>>Entry Name: 2-Nonynoic acid, 9CI, 8CI

ENTRY UNDER REVIEW

CAS Registry Number: 1846-70-4

$\text{H}_3\text{C}(\text{CH}_2)_5\text{C}\equiv\text{CCOOH}$

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: Possesses some antifungal activity

Physical Description: Liq.

Melting Point: Mp -8°

Boiling Point: Bp₁₈ 154-156°. Bp_{2.2} 122°

Rare Chemicals Library: S35402-3

>>Derivative: Me ester

Synonym(s): Methyl octynecarboxylate

CAS Registry Number: 111-80-8

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%

Use/Importance: Possesses some antifungal activity. Used in perfumery

Physical Description: Liq. with violet odour

Boiling Point: Bp_{2.3} 85°

Refractive Index: n_D^{25} 1.4470

Hazard & Toxicity: LD₅₀ (rat, orl) 2220 mg/kg

Aldrich: W27260-4

Rare Chemicals Library: S35314-0

>>Derivative: Amide

Molecular Formula: $\text{C}_9\text{H}_{15}\text{NO}$

Molecular Weight: 153.224

Accurate Mass: 153.115364

Percentage Composition: C 70.55%; H 9.87%; N 9.14%; O 10.44%

Physical Description: Cryst. (Et₂O/petrol)

Melting Point: Mp 94°

>>Derivative: Et ester

Synonym(s): FEMA 2448

CAS Registry Number: 10031-92-2

Molecular Formula: $\text{C}_{11}\text{H}_{18}\text{O}_2$

Molecular Weight: 182.262

Accurate Mass: 182.13068

Percentage Composition: C 72.49%; H 9.95%; O 17.56%

Use/Importance: Flavouring ingredient

Physical Description: Oil

Melting Point: Mp 227°

Density: d^{25} 0.9

Refractive Index: n_D^{20} 1.4517

References: