



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

CAS Registry Number: 1846-70-4
H3C(CH2)5C#CCOOH

Molecular Formula: C9H14O2
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: C10H16O2
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_D²⁵ 1.4470
Hazard & Toxicity: LD₅₀ (rat, orl) 2220 mg/kg

Aldrich: W27260-4
Rare Chemicals Library: S35314-0

>>Derivative: Amide

Molecular Formula: C9H15NO
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: C11H18O2
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: d²⁵ 0.9
Refractive Index: n_D²⁰ 1.4517

References: