



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

ENTRY UNDER REVIEW

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

CAS Registry Number: 1470-50-4

$\text{H}_3\text{C}(\text{CH}_2)_4\text{CH}=\text{CHCOOH}$

Molecular Formula: $\text{C}_8\text{H}_{14}\text{O}_2$

Molecular Weight: 142.197

Accurate Mass: 142.09938

Percentage Composition: C 67.57%; H 9.92%; O 22.50%

>>Variant: (*E*)-form

Synonym(s): FEMA 3957

CAS Registry Number: 1871-67-6

Molecular Formula: $\text{C}_8\text{H}_{14}\text{O}_2$

Molecular Weight: 142.197

Accurate Mass: 142.09938

Percentage Composition: C 67.57%; H 9.92%; O 22.50%

Melting Point: Mp 2°

Boiling Point: Bp₁₂ 135-136°

Aldrich: O-520-9

>>Derivative: Amide

Molecular Formula: $\text{C}_8\text{H}_{15}\text{NO}$

Molecular Weight: 141.213

Accurate Mass: 141.115364

Percentage Composition: C 68.04%; H 10.71%; N 9.92%; O 11.33%

Melting Point: Mp 134.7-135.1°

>>Derivative: Nitrile

Molecular Formula: $\text{C}_8\text{H}_{13}\text{N}$

Molecular Weight: 123.197

Accurate Mass: 123.104799

Percentage Composition: C 78.00%; H 10.64%; N 11.37%

Melting Point: Mp 57.6-58°

Boiling Point: Bp₁₁ 84°

>>Derivative: Me ester

Synonym(s): FEMA 3712

CAS Registry Number: 7367-81-9

Molecular Formula: $\text{C}_9\text{H}_{16}\text{O}_2$

Molecular Weight: 156.224

Accurate Mass: 156.11503

Percentage Composition: C 69.19%; H 10.32%; O 20.48%

Physical Description: Liq.

Boiling Point: Bp₁₂ 80°

Refractive Index: n_D 1.4399

>>Derivative: Et ester

Synonym(s): FEMA 3344

CAS Registry Number: 7367-82-0

Molecular Formula: $\text{C}_{10}\text{H}_{18}\text{O}_2$

Molecular Weight: 170.251

Accurate Mass: 170.13068

Percentage Composition: C 70.55%; H 10.66%; O 18.80%

Physical Description: Liq.

Boiling Point: Bp₁₀ 93-96°

>>Variant: (*Z*)-form