



>>Entry Name: 2-Octenoic acid, 9CI
ENTRY UNDER REVIEW
Synonym(s): 1-Heptene-1-carboxylic acid

CAS Registry Number: 1470-50-4
H3C(CH2)4CH=CHCOOH

Molecular Formula: C8H14O2
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: C8H14O2
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: C8H15NO
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: C8H13N
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: C9H16O2
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: C10H18O2
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