



>>Entry Name: 3-Nonenoic acid, 9Cl, 8Cl

ENTRY UNDER REVIEW

CAS Registry Number: 4124-88-3

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

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%

>>Variant: (*E*)-form

CAS Registry Number: 28163-88-4

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.

Melting Point: Fp -4.4°

Boiling Point: Bp₁ 106°

Solubility: Sol. Et₂O, insol. H₂O

>>Derivative: Me ester

CAS Registry Number: 36781-67-6

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: Bp_{0.5} $69-71^\circ$

>>Derivative: 4-Bromophenacyl ester

Physical Description: Cryst.

Melting Point: Mp $68.2-69.3^\circ$

>>Derivative: Chloride

CAS Registry Number: 764-87-4

Molecular Formula: $\text{C}_9\text{H}_{15}\text{ClO}$

Molecular Weight: 174.67

Accurate Mass: 174.081142

Percentage Composition: C 61.89%; H 8.66%; Cl 20.30%; O 9.16%

Physical Description: Liq.

Boiling Point: Bp_{4.5} $80-81^\circ$

Other Data: Assignment of these props to the *E*-isomer is not certain

>>Derivative: Amide

Molecular Formula: $\text{C}_9\text{H}_{17}\text{NO}$

Molecular Weight: 155.239

Accurate Mass: 155.131014

Percentage Composition: C 69.63%; H 11.04%; N 9.02%; O 10.31%

Physical Description: Cryst. (EtOH)

Melting Point: Mp $74.5-75^\circ$

Other Data: Assignment of these props to the *E*-isomer is not certain

>>Variant: (*Z*)-form

CAS Registry Number: 41653-98-9