



>>Entry Name: 9,12-Octadecadienoic acid, 9CI

ENTRY UNDER REVIEW

CAS Registry Number: 2197-37-7

Related CAS Registry Numbers(s): 3207-50-9 7779-63-7 28984-77-2

$\text{H}_3\text{C}(\text{CH}_2)_4\text{CH}=\text{CHCH}_2\text{CH}=\text{CH}(\text{CH}_2)_7\text{COOH}$

Molecular Formula: $\text{C}_{18}\text{H}_{32}\text{O}_2$

Molecular Weight: 280.45

Accurate Mass: 280.24023

Percentage Composition: C 77.09%; H 11.50%; O 11.41%

Solubility: BERDY SOL: Sol. bases, CHCl_3 , Et_2O ; poorly sol. H_2O , acids

pKa Value: $\text{p}K_{\text{a}}$ 4.77 (25°)

Calculated Log P Data: Log P 7.26 (uncertain value) (calc)

>>Variant: (E,E)-form

Synonym(s): Linolelaidic acid

CAS Registry Number: 506-21-8

Molecular Formula: $\text{C}_{18}\text{H}_{32}\text{O}_2$

Molecular Weight: 280.45

Percentage Composition: C 77.09%; H 11.50%; O 11.41%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 28-29°

Boiling Point: $\text{Bp}_{0.8}$ 179-183°

Solubility: BERDY SOL: Sol. Me_2CO , hexane; poorly sol. H_2O

Sigma: L2156

>>Derivative: Me ester

CAS Registry Number: 2566-97-4

Molecular Formula: $\text{C}_{19}\text{H}_{34}\text{O}_2$

Molecular Weight: 294.476

Accurate Mass: 294.25588

Percentage Composition: C 77.50%; H 11.64%; O 10.87%

Melting Point: Mp -7.8°

Boiling Point: Bp_2 151-152°

Sigma: L2281

Supelco: R47-5215

>>Variant: (9E,12Z)-form

CAS Registry Number: 2420-55-5

Molecular Formula: $\text{C}_{18}\text{H}_{32}\text{O}_2$

Molecular Weight: 280.45

Accurate Mass: 280.24023

Percentage Composition: C 77.09%; H 11.50%; O 11.41%

Source/Synthesis: Obt. by stereomutation of Linoleic acid

Melting Point: Mp 1°

>>Variant: (9Z,12E)-form

CAS Registry Number: 2420-42-0

Molecular Formula: $\text{C}_{18}\text{H}_{32}\text{O}_2$

Molecular Weight: 280.45

Accurate Mass: 280.24023

Percentage Composition: C 77.09%; H 11.50%; O 11.41%

Melting Point: Mp 1°

>>Variant: (Z,Z)-form

Synonym(s): Linoleic acid. Leinolic acid. Telfairic acid. Linolic acid

CAS Registry Number: 60-33-3