



>>Entry Name: 13-Docosenoic acid

Extra CAS Registry Numbers(s): 25378-26-1

Type of Compound Code(s): XA1950

$\text{H}_3\text{C}(\text{CH}_2)_7\text{CH}=\text{CH}(\text{CH}_2)_{11}\text{COOH}$

Molecular Formula: $\text{C}_{22}\text{H}_{42}\text{O}_2$

Molecular Weight: 338.573

Accurate Mass: 338.31848

Percentage Composition: C 78.05%; H 12.50%; O 9.45%

Use/Importance: Antineoplastic agent

Calculated Log P Data: Log P 9.86 (uncertain value) (calc)

>>Variant: (*E*)-form

Synonym(s): Brassidic acid

CAS Registry Number: 506-33-2

Molecular Formula: $\text{C}_{22}\text{H}_{42}\text{O}_2$

Molecular Weight: 338.573

Accurate Mass: 338.31848

Percentage Composition: C 78.05%; H 12.50%; O 9.45%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 61.5°

Boiling Point: Bp₃₀ 282°. Bp₁₀ 256°

Rare Chemicals Library: S42883-3

Sigma: B0884

>>Derivative: Me ester

CAS Registry Number: 7439-44-3

Molecular Formula: $\text{C}_{23}\text{H}_{44}\text{O}_2$

Molecular Weight: 352.599

Accurate Mass: 352.33413

Percentage Composition: C 78.35%; H 12.58%; O 9.08%

Melting Point: Mp 34-35°

Sigma: B8906

>>Derivative: Et ester

CAS Registry Number: 116723-91-2

Molecular Formula: $\text{C}_{24}\text{H}_{46}\text{O}_2$

Molecular Weight: 366.626

Accurate Mass: 366.34978

Percentage Composition: C 78.63%; H 12.65%; O 8.73%

Melting Point: Mp 30.5°

>>Derivative: Nitrile

Molecular Formula: $\text{C}_{22}\text{H}_{41}\text{N}$

Molecular Weight: 319.573

Accurate Mass: 319.323899

Percentage Composition: C 82.69%; H 12.93%; N 4.38%

Melting Point: Mp 22°

Boiling Point: Bp₁₇ 257°

>>Derivative: Anhydride

Molecular Formula: $\text{C}_{44}\text{H}_{82}\text{O}_3$

Molecular Weight: 659.13

Accurate Mass: 658.626395

Percentage Composition: C 80.18%; H 12.54%; O 7.28%

Melting Point: Mp 64°