

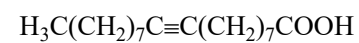


>>Entry Name: 9-Octadecynoic acid, 9Cl

Synonym(s): Stearolic acid

CAS Registry Number: 506-24-1

Related CAS Registry Numbers(s): 1120-32-7



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%

Physical Description: Cryst. (EtOH aq. or EtOH)

Melting Point: Mp 47-48°

Boiling Point: Bp_{1.8} 189-190°

Sigma: S8268

>>Derivative: Et ester

CAS Registry Number: 3343-92-8

Molecular Formula: $\text{C}_{20}\text{H}_{36}\text{O}_2$

Molecular Weight: 308.503

Accurate Mass: 308.27153

Percentage Composition: C 77.87%; H 11.76%; O 10.37%

Boiling Point: Bp₃ 195-197°

>>Derivative: Chloride

CAS Registry Number: 60010-36-8

Molecular Formula: $\text{C}_{18}\text{H}_{31}\text{ClO}$

Molecular Weight: 298.895

Accurate Mass: 298.206342

Percentage Composition: C 72.33%; H 10.45%; Cl 11.86%; O 5.35%

Boiling Point: Bp₁₅ 210°

>>Derivative: Tetrabromide

Synonym(s): 9,9,10,10-Tetrabromooctadecanoic acid

CAS Registry Number: 54288-55-0

Molecular Formula: $\text{C}_{18}\text{H}_{32}\text{Br}_4\text{O}_2$

Molecular Weight: 600.066

Accurate Mass: 595.993574

Percentage Composition: C 36.03%; H 5.37%; Br 53.26%; O 5.33%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 70°

References:

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Hopkins, C.Y. *et al.*, *Tet. Lett.*, 1964, 3011-3013, (*isol, glc*)
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Barve, J.A. *et al.*, *Chem. Phys. Lipids*, 1971, **7**, 311-323, (*synth*)
Frost, D.J. *et al.*, *Chem. Phys. Lipids*, 1975, **15**, 53-85, (*pmr*)
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