



>>Entry Name: 13-Octadecenoic acid

CAS Registry Number: 7378-89-4

Related CAS Registry Numbers(s): 42199-38-2 56338-67-1

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

Molecular Formula: $\text{C}_{18}\text{H}_{34}\text{O}_2$

Molecular Weight: 282.465

Accurate Mass: 282.25588

Percentage Composition: C 76.54%; H 12.13%; O 11.33%

>>Variant: (E)-form

CAS Registry Number: 693-71-0

Molecular Formula: $\text{C}_{18}\text{H}_{34}\text{O}_2$

Molecular Weight: 282.465

Accurate Mass: 282.25588

Percentage Composition: C 76.54%; H 12.13%; O 11.33%

Melting Point: Mp 43.5-44.5°

Sigma: O1883

>>Variant: (Z)-form

CAS Registry Number: 13126-39-1

Molecular Formula: $\text{C}_{18}\text{H}_{34}\text{O}_2$

Molecular Weight: 282.465

Accurate Mass: 282.25588

Percentage Composition: C 76.54%; H 12.13%; O 11.33%

Biological Source: Constit. of various lipid fractions from algae, bacteria, fish and some cooked foods. Also found in various plant spp.

Melting Point: Mp 26.5-27°

Sigma: O9006

>>Derivative: Me ester

CAS Registry Number: 13058-55-4

Molecular Formula: $\text{C}_{19}\text{H}_{36}\text{O}_2$

Molecular Weight: 296.492

Accurate Mass: 296.27153

Percentage Composition: C 76.97%; H 12.24%; O 10.79%

Biological Source: Constit. of *Aesculus indica*

Physical Description: Liq.

Boiling Point: Bp_{0.4} 145°

Sigma: O9256

Supelco: R47-4445

>>Derivative: Et ester

CAS Registry Number: 101766-90-9

Molecular Formula: $\text{C}_{20}\text{H}_{38}\text{O}_2$

Molecular Weight: 310.519

Accurate Mass: 310.28718

Percentage Composition: C 77.36%; H 12.33%; O 10.30%

Biological Source: Constit. of *Aesculus indica*

Physical Description: Viscous liq.

References:

Gunstone, F.D. *et al.*, *Chem. Phys. Lipids*, 1967, **1**, 209; 264; 1977, **18**, 115, (*synth, cmr*)

Barve, J.A. *et al.*, *Chem. Phys. Lipids*, 1971, **7**, 311, (*synth*)

Singh, B. *et al.*, *J. Nat. Prod.*, 1989, **52**, 180, (*isol, ir, pmr, cmr, esters*)

Subbaraman, A.S. *et al.*, *Indian J. Chem., Sect. B*, 1991, **30**, 865, (*synth, ir*)