



>>Entry Name: 11-Eicosenoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 11-Icosenoic acid

CAS Registry Number: 2462-94-4

Extra CAS Registry Numbers(s): 26764-41-0

$\text{H}_3\text{C}(\text{CH}_2)_7\text{CH}=\text{CH}(\text{CH}_2)_9\text{COOH}$

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%

>>Variant: (E)-form

CAS Registry Number: 62322-84-3

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%

Melting Point: Mp 49-51°

>>Variant: (Z)-form

Synonym(s): Gondoic acid

CAS Registry Number: 5561-99-9

Extra CAS Registry Numbers(s): 28933-89-3

Type of Compound Code(s): VA0600

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 rape oil and fish oils as glyceride. Also in other plant oils, eg. false flax (*Camelina sativa*), and swede (*Brassica napobrassica*)

Physical Description: Cryst. (Me_2CO /hexane)

Melting Point: Mp 24-25°

Aldrich: 28571-4

Sigma: E5751

>>Derivative: Me ester

CAS Registry Number: 2390-09-2

Molecular Formula: $\text{C}_{21}\text{H}_{40}\text{O}_2$

Molecular Weight: 324.546

Accurate Mass: 324.30283

Percentage Composition: C 77.72%; H 12.42%; O 9.86%

Melting Point: Mp -45°

Aldrich: 28572-2

Sigma: E5876

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 783C; 988B, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 686A, (*ir*)

Fieser, L.F. *et al.*, *J.A.C.S.*, 1948, **70**, 71, (*synth*)

Argoudelis, C.J. *et al.*, *Lipids*, 1968, **3**, 379, (*struct, ms*)

Karrer, W. *et al.*, *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 742, (*occur*)

Spencer, F. *et al.*, *Chem. Phys. Lipids*, 1973, **11**, 215, (*synth*)