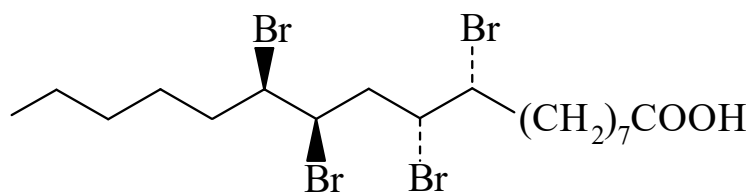




>>Entry Name: **9,10,12,13-Tetrabromooctadecanoic acid**

Synonym(s): Linoleic acid tetrabromide. 9,10,12,13-Tetrabromostearic acid



(9*RS*,10*RS*,12*RS*,13*RS*)-form

CAS Registry Number: 1794-89-4

Molecular Formula: C₁₈H₃₂Br₄O₂

Molecular Weight: 600.066

Accurate Mass: 595.993574

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

Rare Chemicals Library: S37158-0

>>Variant: (9*RS*,10*RS*,12*RS*,13*RS*)-form

CAS Registry Number: 56846-03-8

Molecular Formula: C₁₈H₃₂Br₄O₂

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. (Et₂O/petrol)

Melting Point: Mp 114.7-115.2°

>>Derivative: Me ester

Molecular Formula: C₁₉H₃₄Br₄O₂

Molecular Weight: 614.092

Accurate Mass: 610.009224

Percentage Composition: C 37.16%; H 5.58%; Br 52.05%; O 5.21%

Physical Description: Cryst.

Melting Point: Mp 63° (50-56°)

>>Derivative: Et ester

Molecular Formula: C₂₀H₃₆Br₄O₂

Molecular Weight: 628.119

Accurate Mass: 624.024874

Percentage Composition: C 38.24%; H 5.78%; Br 50.88%; O 5.09%

Physical Description: Cryst.

Melting Point: Mp 63° (58-58.5°)

>>Variant: (9*RS*,10*RS*,12*SR*,13*SR*)-form

CAS Registry Number: 56846-04-9

Molecular Formula: C₁₈H₃₂Br₄O₂

Molecular Weight: 600.066

Accurate Mass: 595.993574

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

Source/Synthesis: From bromination of linoleic acid

Physical Description: Oil

References:

Org. Synth., 1942, **22**, 76, (*synth*)

Olson, E.S., *J. Am. Oil Chem. Soc.*, 1975, **52**, 319, (*stereochem, nmr*)

Carman, R.M. *et al.*, *Aust. J. Chem.*, 1995, **48**, 1495, (*cryst struct*)