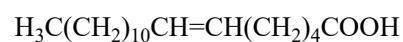




>>Entry Name: 6-Octadecenoic acid



Molecular Formula: C₁₈H₃₄O₂

Molecular Weight: 282.465

Accurate Mass: 282.25588

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

>>Variant: (*E*)-form

Synonym(s): Petroselaidic acid. Tarelaidinic acid

CAS Registry Number: 593-40-8

Molecular Formula: C₁₈H₃₄O₂

Molecular Weight: 282.465

Accurate Mass: 282.25588

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

Biological Source: Minor constit. of plant oils accompanying the major *Z*-isomer

Physical Description: Cryst. (CHCl₃ or MeOH)

Melting Point: Mp 52.7-53.4°. Mp 54-59°

Sigma: P4776

>>Derivative: Me ester

CAS Registry Number: 14620-36-1

Molecular Formula: C₁₉H₃₆O₂

Molecular Weight: 296.492

Accurate Mass: 296.27153

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

Boiling Point: Bp₁₀ 208-210°. Bp₄ 185-186°

>>Derivative: Chloride

Molecular Formula: C₁₈H₃₃ClO

Molecular Weight: 300.911

Accurate Mass: 300.221992

Percentage Composition: C 71.85%; H 11.05%; Cl 11.78%; O 5.32%

Boiling Point: Bp₂ 144-146°

>>Variant: (*Z*)-form

Synonym(s): Petroselinic acid

CAS Registry Number: 593-39-5

Molecular Formula: C₁₈H₃₄O₂

Molecular Weight: 282.465

Accurate Mass: 282.25588

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

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

Melting Point: Mp 33°

Boiling Point: Bp_{2.5} 215-217° (lit. gives a pressure range). Bp_{0.15} 148-152°

Sigma: P8750

References:

Baker, B.W. *et al.*, *J.C.S.*, 1952, 1804

Lamb, P.B. *et al.*, *J.C.S.*, 1952, 5032, (*synth, config*)

Swern, D. *et al.*, *J. Am. Oil Chem. Soc.*, 1955, **32**, 539, (*cryst struct*)

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

Batchelor, J.G. *et al.*, *J.O.C.*, 1974, **39**, 1698, (*cmr*)

Parodi, P.W., *J. Dairy Sci.*, 1976, **59**, 1870, (*synth, glc*)

Saito, Y. *et al.*, *Biochim. Biophys. Acta*, 1978, **529**, 224

Conacher, H.B.S. *et al.*, *J. Assoc. Off. Anal. Chem.*, 1978, **61**, 702, (*glc*)

Kaneko, F. *et al.*, *Acta Cryst. C*, 1992, **48**, 1054; 1057, (*cryst struct*)

Cahoon, E.B. *et al.*, *Prog. Lipids Res.*, 1994, **33**, 155, (*rev, biosynth*)