



>>Entry Name: 16-Methyloctadecanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 16-Methylstearic acid. Anteisononadecanoic acid

CAS Registry Number: 17001-28-4

Related CAS Registry Numbers(s): 59992-30-2 73641-06-2

$\text{H}_3\text{CCH}_2\text{CH}(\text{CH}_3)(\text{CH}_2)_{14}\text{COOH}$

Molecular Formula: $\text{C}_{19}\text{H}_{38}\text{O}_2$

Molecular Weight: 298.508

Accurate Mass: 298.28718

Percentage Composition: C 76.45%; H 12.83%; O 10.72%

Biological Source: Occurs in butterfat, several woods, tobacco and Baltic salmon

Melting Point: Mp 49.9-50.6°

Other Data: The natural compd. is probably enantiomeric

>>Derivative: Me ester

CAS Registry Number: 2490-16-6

Molecular Formula: $\text{C}_{20}\text{H}_{40}\text{O}_2$

Molecular Weight: 312.535

Accurate Mass: 312.30283

Percentage Composition: C 76.86%; H 12.90%; O 10.24%

Biological Source: Occurs in *Staphylococcus aureus* membrane

Boiling Point: Bp_{1.2} 176°

>>Derivative: Amide

Molecular Formula: $\text{C}_{19}\text{H}_{39}\text{NO}$

Molecular Weight: 297.523

Accurate Mass: 297.303164

Percentage Composition: C 76.70%; H 13.21%; N 4.71%; O 5.38%

Melting Point: Mp 93.2°

References:

Cason, J. *et al.*, *J.A.C.S.*, 1944, **66**, 46

Abrahamsson, S., *Acta Cryst.*, 1958, **11**, 270, (*cryst struct*)

Fischmeister, I., *Ark. Kemi*, 1963, **20**, 353, (*ir*)

Silvius, J.R. *et al.*, *Chem. Phys. Lipids*, 1980, **26**, 67

Jensen, N.J. *et al.*, *Lipids*, 1986, **21**, 362, (*ms*)