



>>Entry Name: 12-Oxooctadecanoic acid

Synonym(s): 12-Oxostearic acid. Lycaonic acid

CAS Registry Number: 925-44-0

$\text{H}_3\text{C}(\text{CH}_2)_5\text{CO}(\text{CH}_2)_{10}\text{COOH}$

Molecular Formula: $\text{C}_{18}\text{H}_{34}\text{O}_3$

Molecular Weight: 298.465

Accurate Mass: 298.250795

Percentage Composition: C 72.44%; H 11.48%; O 16.08%

Melting Point: Mp 81.5°

>>Derivative: Semicarbazone

Melting Point: Mp 122°

>>Derivative: Me ester

CAS Registry Number: 2380-27-0

Molecular Formula: $\text{C}_{19}\text{H}_{36}\text{O}_3$

Molecular Weight: 312.492

Accurate Mass: 312.266445

Percentage Composition: C 73.03%; H 11.61%; O 15.36%

Melting Point: Mp 46-48°

Boiling Point: Bp_{0.8} 178-180°

Aldrich: 30335-6

>>Derivative: Pyrrolidide

Synonym(s): Lycaonic acid pyrrolidide. 1-(1,12-Dioxooctadecyl)pyrrolidine

CAS Registry Number: 83182-47-2

Molecular Formula: $\text{C}_{22}\text{H}_{41}\text{NO}_2$

Molecular Weight: 351.571

Accurate Mass: 351.313729

Percentage Composition: C 75.16%; H 11.75%; N 3.98%; O 9.10%

Biological Source: Alkaloid from the roots of *Achillea* spp. (Compositae)

Melting Point: Mp 44°

>>Derivative: Piperidide

Synonym(s): Lycaonic acid piperidide. 1-(1,12-Dioxooctadecyl)piperidine

CAS Registry Number: 83182-45-0

Molecular Formula: $\text{C}_{23}\text{H}_{43}\text{NO}_2$

Molecular Weight: 365.598

Accurate Mass: 365.329379

Percentage Composition: C 75.56%; H 11.85%; N 3.83%; O 8.75%

Biological Source: Alkaloid from the roots of *Achillea lycaonica* (Compositae)

Melting Point: Mp 41°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 1105C, (*nmr*)
Belopol'skii, M.P. *et al.*, *CA*, 1937, **31**, 7397, (*synth*)
Tulloch, A.P., *Can. J. Chem.*, 1977, **55**, 1135, (*cmr*)
Tulloch, A.P. *et al.*, *Lipids*, 1977, **12**, 92, (*synth*)
Greger, H. *et al.*, *Phytochemistry*, 1982, **21**, 1071, (*isol, ir, pmr, struct, pyrrolidide, piperidide*)
Bohlmann, F. *et al.*, *Tetrahedron*, 1983, **39**, 123, (*synth*)
Dasaradlin, L. *et al.*, *J.C.S. Perkin 2*, 1995, 221, (*Me ester, synth*)