



>>Entry Name: 9-Octadecenylamine, 8Cl

Synonym(s): 9-Octadecen-1-amine, 9Cl. 1-Amino-9-octadecene

CAS Registry Number: 1838-19-3

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

Molecular Formula:  $\text{C}_{18}\text{H}_{37}\text{N}$

Molecular Weight: 267.497

Accurate Mass: 267.292599

Percentage Composition: C 80.82%; H 13.94%; N 5.24%

Calculated Log P Data: Log P 7.84 (uncertain value) (calc)

>>Derivative: Hydrofluoride

Synonym(s): Dectaflur, INN. SKF 38094

CAS Registry Number: 36505-83-6

Use/Importance: Dental caries prophylactic

Development Status: Never marketed

>>Variant: (E)-form

Synonym(s): Elaidylamine

Molecular Formula:  $\text{C}_{18}\text{H}_{37}\text{N}$

Molecular Weight: 267.497

Accurate Mass: 267.292599

Percentage Composition: C 80.82%; H 13.94%; N 5.24%

Physical Description: Cryst.

Melting Point: Mp 39°

Boiling Point: Bp<sub>2</sub> 149°

>>Derivative: Picrate

Melting Point: Mp 89.5°

>>Variant: (Z)-form

Synonym(s): Oleylamine

CAS Registry Number: 112-90-3

Molecular Formula:  $\text{C}_{18}\text{H}_{37}\text{N}$

Molecular Weight: 267.497

Accurate Mass: 267.292599

Percentage Composition: C 80.82%; H 13.94%; N 5.24%

Physical Description: Oil

Melting Point: Mp 25° (21°)

Boiling Point: Bp<sub>2</sub> 147°

Aldrich: O-780-5

Fluka: 75350

>>Derivative: Picrate

Melting Point: Mp 76.4°

#### References:

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 519A, (nmr)

*Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **1**, 323B, (ir)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 413B, (ir, Z-form)

Ucciani, E. *et al.*, *Chem. Phys. Lipids*, 1968, **2**, 240; 256, (synth, pmr)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, OHM700