



>>Entry Name: 1-Hexadecylamine

Synonym(s): 1-Hexadecanamine, 9Cl. 1-Aminohexadecane. Cetylamine

CAS Registry Number: 143-27-1

$\text{H}_3\text{C}(\text{CH}_2)_{14}\text{CH}_2\text{NH}_2$

Molecular Formula: $\text{C}_{16}\text{H}_{35}\text{N}$

Molecular Weight: 241.459

Accurate Mass: 241.276949

Percentage Composition: C 79.59%; H 14.61%; N 5.80%

Melting Point: Mp 46.2°

Boiling Point: Bp_{5,2} 162-165°

pKa Value: pK_a 10.61 (25°)

Calculated Log P Data: Log P 7.27 (uncertain value) (calc)

Hazard & Toxicity: LD₅₀ (mus, ipr) 200 mg/kg. Exp. reprod. and teratogenic effects

Aldrich: 44531-2

Fluka: 52300

>>Derivative: Hydrofluoride

Synonym(s): Hetaflur, BAN, INN, USAN. GA 242. SKF 2208

CAS Registry Number: 3151-59-5

Use/Importance: Dental caries prophylactic

Development Status: Never marketed

Hazard & Toxicity: Exp. reprod. and teratogenic effects. LD₅₀ (mus, ipr) approx. 45 mg/kg

>>Derivative: Hydrochloride

CAS Registry Number: 1602-97-7

Melting Point: Mp 178°

>>Derivative: *N*-Ac

CAS Registry Number: 14303-96-9

Molecular Formula: $\text{C}_{18}\text{H}_{37}\text{NO}$

Molecular Weight: 283.496

Accurate Mass: 283.287514

Percentage Composition: C 76.26%; H 13.15%; N 4.94%; O 5.64%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 71°

>>Derivative: *N,N*-Di-Me

CAS Registry Number: 112-69-6

Molecular Formula: $\text{C}_{18}\text{H}_{39}\text{N}$

Molecular Weight: 269.513

Accurate Mass: 269.308249

Percentage Composition: C 80.22%; H 14.58%; N 5.20%

Boiling Point: Bp₂ 135-136°

Fluka: 40460

>>Derivative: *N,N*-Di-Me, N-oxide

CAS Registry Number: 7128-91-8

Molecular Formula: $\text{C}_{18}\text{H}_{39}\text{NO}$

Molecular Weight: 285.512

Accurate Mass: 285.303164

Percentage Composition: C 75.72%; H 13.77%; N 4.91%; O 5.60%

Melting Point: Mp 163° (as hydrochloride)

References: