



>>Entry Name: Acetylcholine(1+)

Synonym(s): 2-Acetyloxy-*N,N,N*-trimethylethanaminium, 9Cl. Choline acetate

CAS Registry Number: 51-84-3

$\text{Me}_3\text{N}^{(+)}\text{CH}_2\text{CH}_2\text{OAc}$

Molecular Formula: $\text{C}_7\text{H}_{16}\text{NO}_2^{(+)}$

Molecular Weight: 146.209

Accurate Mass: 146.118104

Percentage Composition: C 57.50%; H 11.03%; N 9.58%; O 21.89%

Biological Source: Occurs in blood, spleen, ergot and plants and in brain tissue in complexed form eg. in ergot and *Capsella bursa-pastoris* (Cruciferae)

Biological Use/Importance: Neurotransmitter, cholinergic and miotic agent, cardiac depressant, peripheral vasodilator

Other Data: Easily hyd. by alkalis, and *in vivo* by cholinesterases

>>Derivative: Chloride

Synonym(s): Acetylcholine chloride, BAN, INN, USAN. Miochol. Ovisot

CAS Registry Number: 60-31-1

Molecular Formula: $\text{C}_7\text{H}_{16}\text{ClNO}_2$

Molecular Weight: 181.662

Accurate Mass: 181.086956

Percentage Composition: C 46.28%; H 8.88%; Cl 19.52%; N 7.71%; O 17.61%

Physical Description: V. deliquescent cryst. powder

Melting Point: Mp 149-152°

Solubility: BERDY SOL: Sol. H_2O

Hazard & Toxicity: LD₅₀ (rat, orl) 2500 mg/kg. LD₅₀ (rat, ivn) 22 mg/kg

Aldrich: 13535-6

Fluka: 1020

Sigma: A6750

>>Derivative: Bromide

CAS Registry Number: 66-23-9

Molecular Formula: $\text{C}_7\text{H}_{16}\text{BrNO}_2$

Molecular Weight: 226.113

Accurate Mass: 225.05644

Percentage Composition: C 37.18%; H 7.13%; Br 35.34%; N 6.19%; O 14.15%

Physical Description: Deliquescent prisms (EtOH)

Melting Point: Mp 143°

Aldrich: 85968-0

Fluka: 1010

Sigma: A6500

>>Derivative: Iodide

CAS Registry Number: 2260-50-6

Molecular Formula: $\text{C}_7\text{H}_{16}\text{INO}_2$

Molecular Weight: 273.113

Accurate Mass: 273.022577

Percentage Composition: C 30.78%; H 5.90%; I 46.47%; N 5.13%; O 11.72%

Melting Point: Mp 161°

Aldrich: 10043-9

Fluka: 1030

Sigma: A7000

References: