



>>Entry Name: Bethanechol(1+)

Synonym(s): 2-[(Aminocarbonyl)oxy]-*N,N,N*-trimethyl-1-propanaminium, 9Cl. (2-Hydroxypropyl)trimethylammonium carbamate, 8Cl. Carbamylmethylcholine

CAS Registry Number: 674-38-4

Related CAS Registry Numbers(s): 111244-96-3 111244-97-4 111318-31-1

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

Molecular Formula: $\text{C}_7\text{H}_{17}\text{N}_2\text{O}_2^{(+)}$

Molecular Weight: 161.223

Accurate Mass: 161.129003

Percentage Composition: C 52.15%; H 10.63%; N 17.38%; O 19.85%

>>Variant: (±)-form

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Molecular Weight: 161.223

Accurate Mass: 161.129003

Percentage Composition: C 52.15%; H 10.63%; N 17.38%; O 19.85%

>>Derivative: Chloride

Synonym(s): Bethanecol chloride, BAN, JAN, Duvoid, Urecholine, Myocholine, Mictone, Urocarb. Many other names

CAS Registry Number: 590-63-6

Molecular Formula: $\text{C}_7\text{H}_{17}\text{ClN}_2\text{O}_2$

Molecular Weight: 196.676

Accurate Mass: 196.097855

Percentage Composition: C 42.75%; H 8.71%; Cl 18.03%; N 14.24%; O 16.27%

Use/Importance: Cholinergic agent, muscarinic agonist. Used to promote bladder emptying

Physical Description: Hygroscopic cryst. with sl. amine odour

Melting Point: Mp 218-219 dec.°

Solubility: V. sol. H_2O

pKa Value: pK_a 5.5-6.5 (H_2O)

Hazard & Toxicity: LD₅₀ (rat, orl) 1500 mg/kg. LD₅₀ (rat, ivn) 21 mg/kg. Long-term administration to rats (14d, ipr) caused pancreatic hypertrophy

Sigma: C5259

References:

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