



>>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

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>>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:

- U.S. Pat., 1943, Merck, 2 322 375; CA, **38**, 2208, (synth, pharmacol)
La Barre, J., Arch. Int. Pharmacodyn. Ther., 1957, **109**, 229, (pharmacol)
Cerri, O. et al., Pharm. Acta Helv., 1959, **34**, 13, (anal)
Partington, P. et al., Mol. Pharmacol., 1972, **8**, 269, (nmr)
Coutls, R.T., J. Pharm. Sci., 1973, **62**, 769, (ms)
Finkbeiner, A.E., J. Urol. (Baltimore), 1985, **134**, 443, (pharmacol, rev)
Megens, A.A.H.P. et al., Arzneim.-Forsch., 1991, **41**, 631, (pharmacol)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1112
Kato, M. et al., Eur. J. Pharmacol., 1994, **292**, 47, (pharmacol)
Negwer, M., Organic-Chemical Drugs and their Synonyms, 7th edn., Akademie-Verlag, 1994, 936
Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, HOA500