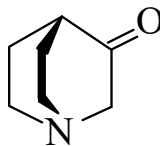




>>Entry Name: 1-Azabicyclo[2.2.2]octan-3-one, 9Cl

Synonym(s): 3-Quinuclidone, 8Cl. 3-Quinuclidinone



CAS Registry Number: 3731-38-2

Related CAS Registry Numbers(s): 137239-14-6 157127-50-9 157127-51-0

Molecular Formula: C₇H₁₁NO

Molecular Weight: 125.17

Accurate Mass: 125.084064

Percentage Composition: C 67.17%; H 8.86%; N 11.19%; O 12.78%

>>Derivative: Hydrochloride

CAS Registry Number: 1193-65-3

Physical Description: Prisms (2-propanol)

Melting Point: Mp 294-296° (311-313° dec.)

Fluka: 22711

>>Derivative: Oxime

CAS Registry Number: 35423-17-7

Molecular Formula: C₇H₁₂N₂O

Molecular Weight: 140.185

Accurate Mass: 140.094963

Percentage Composition: C 59.98%; H 8.63%; N 19.98%; O 11.41%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 117-119°

>>Derivative: O-Methyloxime; hydrochloride

Synonym(s): 3-Methoxyiminoquinuclidinium chloride. Org 32763

CAS Registry Number: 147760-19-8

Molecular Formula: C₈H₁₅ClN₂O

Molecular Weight: 190.672

Accurate Mass: 190.08729

Percentage Composition: C 50.39%; H 7.93%; Cl 18.59%; N 14.69%; O 8.39%

Biological Use/Importance: Muscarinic agonist. Possible use in cholinergic replacement therapy for Alzheimer's disease

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 720B, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 462B, (*ir*)
Sternbach, L.H. *et al.*, *J.A.C.S.*, 1952, **74**, 2215, (*synth*)
Grob, C.A. *et al.*, *Helv. Chim. Acta*, 1963, **46**, 2658, (*synth*)
Rubstov, M.V. *et al.*, *Zh. Obshch. Khim.*, 1964, **34**, 2222
Kostyanovsky, R.G. *et al.*, *Org. Mass Spectrom.*, 1970, **3**, 1023, (*ms*)
v. Binst, G. *et al.*, *Org. Magn. Reson.*, 1972, **4**, 625, (*cmr*)
Org. Synth., Coll. Vol., 5, 1973, 989
Vorob'eva, V.Ya. *et al.*, *CA*, 1979, **91**, 175164n, (*synth*)
Eur. Pat., 1991, *Warner-Lambert*, 445 731; *CA*, **116**, 6419d, (*synth, pharmacol, deriv*)
de Costa, B.R. *et al.*, *J. Med. Chem.*, 1993, **36**, 2311, (*oxime, synth, pmr*)
Schouten, A. *et al.*, *Acta Cryst. C*, 1994, **50**, 128, (*cryst struct, deriv*)