



>>Entry Name: 3-Amino-4-chlorobenzoic acid, 9Cl, 8Cl

CAS Registry Number: 2840-28-0

Molecular Formula: $C_7H_6ClNO_2$

Molecular Weight: 171.583

Accurate Mass: 171.008706

Percentage Composition: C 49.00%; H 3.52%; Cl 20.66%; N 8.16%; O 18.65%

Use/Importance: Has herbicidal props.

Physical Description: Needles

Melting Point: Mp 212-215°

Aldrich: 23936-4

Fluka: 7370

>>Derivative: Me ester

CAS Registry Number: 40872-87-5

Molecular Formula: $C_8H_8ClNO_2$

Molecular Weight: 185.609

Accurate Mass: 185.024356

Percentage Composition: C 51.77%; H 4.34%; Cl 19.10%; N 7.55%; O 17.24%

Melting Point: Mp 82-83°

>>Derivative: N-Ac

CAS Registry Number: 101870-46-6

Molecular Formula: $C_9H_8ClNO_3$

Molecular Weight: 213.62

Accurate Mass: 213.019271

Percentage Composition: C 50.60%; H 3.77%; Cl 16.60%; N 6.56%; O 22.47%

Melting Point: Mp 133°. Mp 265°

>>Derivative: 2-(Dimethylamino)ethyl ester

Synonym(s): Clormecaine, INN. Rec 1/0060

CAS Registry Number: 13930-34-2

Molecular Formula: $C_{11}H_{15}ClN_2O_2$

Molecular Weight: 242.704

Accurate Mass: 242.082205

Percentage Composition: C 54.44%; H 6.23%; Cl 14.61%; N 11.54%; O 13.18%

Use/Importance: Local anaesthetic

Melting Point: Mp 171-173°

Calculated Log P Data: Log P 2.1 (calc)

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **2**, 217D, (*ir*)
Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 1119A, (*nmr*)
Setnikar, I. *et al.*, *Boll. Chim. Farm.*, 1958, **97**, 457-480, (*pharmacol*)
Da Re, P. *et al.*, *Farmaco, Ed. Sci.*, 1958, **13**, 574-578, (*synth, clormecaine*)
Mehta, V.K. *et al.*, *J. Indian Chem. Soc.*, 1959, **36**, 99-102, (*synth*)
Filleux-Blanchard, M.C. *et al.*, *Org. Magn. Reson.*, 1973, **5**, 221-225, (*pmr*)
Baruffini, A. *et al.*, *CA*, 1978, **89**, 1598, (*use*)
Mossi, W. *et al.*, *Helv. Chim. Acta*, 1992, **75**, 2531-2537, (*N-Ac, synth, ir, pmr, cmr*)