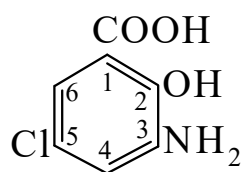




>>Entry Name: 3-Amino-5-chloro-2-hydroxybenzoic acid, 9Cl

Synonym(s): 3-Amino-5-chlorosalicylic acid, 8Cl



CAS Registry Number: 7180-80-5

Molecular Formula: C₇H₆ClNO₃

Molecular Weight: 187.582

Accurate Mass: 187.003621

Percentage Composition: C 44.82%; H 3.22%; Cl 18.90%; N 7.47%; O 25.59%

Use/Importance: Has antiinflammatory activity

Melting Point: Mp 240 dec.°

>>Derivative: N-Ac

Molecular Formula: C₉H₈ClNO₄

Molecular Weight: 229.619

Accurate Mass: 229.014186

Percentage Composition: C 47.08%; H 3.51%; Cl 15.44%; N 6.10%; O 27.87%

Melting Point: Mp 291°

>>Derivative: Me ester

CAS Registry Number: 5043-81-2

Molecular Formula: C₈H₈ClNO₃

Molecular Weight: 201.609

Accurate Mass: 201.019271

Percentage Composition: C 47.66%; H 4.00%; Cl 17.58%; N 6.95%; O 23.81%

Physical Description: Pale yellow cryst.

Melting Point: Mp 92-93°

>>Derivative: Me ether, nitrile

Synonym(s): 3-Amino-5-chloro-2-methoxybenzonitrile

Molecular Formula: C₈H₇ClN₂O

Molecular Weight: 182.609

Accurate Mass: 182.02469

Percentage Composition: C 52.62%; H 3.86%; Cl 19.41%; N 15.34%; O 8.76%

Physical Description: Cryst. (hexane/EtOAc)

References:

Plessing, C.B., *CA*, 1966, **64**, 6555, (*synth*)

Martin, N. *et al.*, *CA*, 1972, **76**, 68096, (*use*)

Lin, C.-T. *et al.*, *J.C.S. Perkin 2*, 1978, 957-962, (*synth, pmr*)

Kawakita, T. *et al.*, *Chem. Pharm. Bull.*, 1992, **40**, 624-630, (*Me ester, synth, ir, pmr*)

Suzuki, T. *et al.*, *Chem. Pharm. Bull.*, 1999, **47**, 120-122, (*Me ether nitrile, synth, pmr*)