



>>Entry Name: 2-Amino-4-bromobenzoic acid, 9Cl

Synonym(s): 4-Bromoanthranilic acid, 8Cl

CAS Registry Number: 20776-50-5

Molecular Formula: $C_7H_6BrNO_2$

Molecular Weight: 216.034

Accurate Mass: 214.97819

Percentage Composition: C 38.92%; H 2.80%; Br 36.99%; N 6.48%; O 14.81%

Physical Description: Needles

Melting Point: Mp 222°

pKa Value: pK_{a1} 1.24; pK_{a2} 4.37 (25°, 0.1M KCl)

>>Derivative: Me ester

Molecular Formula: $C_8H_8BrNO_2$

Molecular Weight: 230.061

Accurate Mass: 228.99384

Percentage Composition: C 41.77%; H 3.50%; Br 34.73%; N 6.09%; O 13.91%

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 78°

>>Derivative: N-Ac

Molecular Formula: $C_9H_8BrNO_3$

Molecular Weight: 258.071

Accurate Mass: 256.988755

Percentage Composition: C 41.89%; H 3.12%; Br 30.96%; N 5.43%; O 18.60%

Melting Point: Mp 217°

References:

Friedlander, P. *et al.*, *Annalen*, 1912, **388**, 23, (*synth*)

Frejka, J. *et al.*, *Coll. Czech. Chem. Comm.*, 1935, **7**, 436, (*synth*)

Boojamra, C.G. *et al.*, *J.O.C.*, 1997, **62**, 1240-1256, (*synth*)