



>>Entry Name: 2-Amino-5-bromobenzoic acid, 9CI

Synonym(s): 5-Bromoanthranilic acid, 8CI

CAS Registry Number: 5794-88-7

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 219-220°

pKa Value: pK_{a1} 1.6; pK_{a2} 4.41 (25°, 0.1M KCl)

Aldrich: 26011-8

Fluka: 7145

>>Derivative: Me ester

CAS Registry Number: 52727-57-8

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%

Melting Point: Mp 74°

>>Derivative: N-Ac

CAS Registry Number: 38985-79-4

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 227-228°

>>Derivative: Amide

CAS Registry Number: 16313-66-9

Molecular Formula: $C_7H_7BrN_2O$

Molecular Weight: 215.049

Accurate Mass: 213.994174

Percentage Composition: C 39.10%; H 3.28%; Br 37.16%; N 13.03%; O 7.44%

Melting Point: Mp 177°

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 1120C, (*nmr*)

Wheeler, A.S. *et al.*, *J.A.C.S.*, 1910, **32**, 770, (*synth*)

Freundler, P., *Bull. Soc. Chim. Fr.*, 1911, **9**, 607, (*synth*)

Leiby, R.W., *J.O.C.*, 1985, **50**, 2926, (*synth*)